Plenary I: AEESP Lecture

From Particle Counting to Aerosol Collection: Just Add Water. SUSANNE HERING, *Aerosol Dynamics Inc.*

Ultrafine, airborne particles are important in the atmosphere, and in some industrial processes. Yet direct measurement is difficult, as most are too small to detect optically, or to collect inertially. Since the nineteenth century, aerosol scientists have circumvented this issue using condensational growth to enlarge ultrafine particles. Today, applications extend from number concentration measurements, to collection for chemical analysis, to aerodynamic concentration for mass spectrometry or exposure studies.

Although the original, adiabatic expansion methods of Aitken and Courtier used water as the condensing species, the more wide-spread method since the 1970s has been laminar-flow, alcohol-based condensational growth. The continuous flow and single particle counting capability of these methods is important to many applications, but the alcohol is not always suitable. The desire to return to water as the condensing material, without sacrificing the advantages of the alcohol systems, motivated the development of the laminar-flow water condensation particle counter (water-CPC). The challenge is the high diffusivity of water vapor. The water-CPC reverses the temperatures of the laminar flow alcohol instruments, with a cold saturator followed by a warm, wet-walled condenser. This approach recognizes that condensation is not created by a cold region, but rather is a result of the relative rates of thermal and vapor diffusion. Water, being the smaller molecule, has a mass diffusivity that is larger than the thermal diffusivity of air. As a cooled flow enters the warm, wet walled region, both heat and water vapor diffuse into the flow; yet the water vapor wins the race, creating a region of high supersaturation along the centerline. This approach readily activates condensational growth at 5 nm. However, as originally implemented, the output flow that is warm and humid, forcing optics to be operated at elevated temperature, and compromising volatile species collected for chemical analysis.

A new, “moderated” approach eliminates the warm, humid output flow. The uniformly warm, wet-walled condensing region of the original approach is replaced by a short, warm wet-walled, “initiator” section followed by a somewhat longer cold, “moderator” section. Once the vapor supersaturation is created within the wet-, warm-walled initiator region, the saturation profiles are insensitive to the temperature of the walls downstream. The subsequent moderator section can be operated the same temperature as the initiator (as done in the first water-CPCs), or at a colder temperature, with no affect on the peak supersaturation. But with the cold moderator the temperature and dew point of the output flow are below 20°C, and non-condensing at typical room temperature.

This “moderated” method opens the door to many additional applications. It is possible to collect ambient aerosol in a concentrated, dry 1-mm diameter spot without heating the sample above ambient temperatures. The approach can be used for directly imaging particles within a mobility separation column, without fogging the optics, enabling fast size distributions, or rapid determination of hygroscopic growth. With the moderated approach, the output temperature is not longer coupled the temperature of the warm initiator section, and thus the system can be operated at high temperature differences between the first two stages, enabling the detection of particles in the 1-2 nm size range. Moreover, it possible to control the output relative humidity to the same value as the that of a conditioned sampled air stream, creating a reservoir-less system that operates for weeks without replenishing the wick. Collection and counting can be combined in a single unit – making self-sustaining condensation counter-collector, such that every particle once counted is deposited on a small substrate that may be removed for microscopic or micro-chemical analysis. These are some of the various applications of water-based condensational growth to aerosol measurement.

Keywords: nanoparticle, condensation particle collector, electrical charging, particle imaging

Plenary II: Friedlander Lecture

Industrialization of Fine-Particle-Based “Products by Process” to Enable Demanding Customer Applications. YAKOV KUTSOVSKY, *Cabot Corporation*

Over the last 150 years, aerosol-produced fine particles have been used to enable key everyday applications – newspaper printing and reinforcement of tires with carbon black, chemical mechanical polishing of silicon wafers and silicone reinforcement with fumed metal oxides. In contrast, current trends in modern society require vehicle light-weighting and electrification, digital ink jet printing and 3D additive manufacturing. These trends place high demands on new materials that need to deliver key performance attributes as well as scaled manufacturing to allow the appropriate cost-in-use in the applications.

Development and scale-up of particles with the desired application performance attributes bring product and process needs together to define the concept of “product by process” - materials characteristics and performance that are defined by the particle production process and scale. This presentation will introduce this concept and will provide several examples of how it is applied in development of new products for tires and energy materials applications. These developments show that the connection between application needs and a deep understanding of material properties to deliver them can enable new innovations in century old technologies.

In addition to expanding opportunities with existing classes of materials such as carbon blacks we are advancing process and applications technologies with advanced carbon materials - graphenes and carbon nanostructures. These materials require a holistic approach spanning safe production and uses of these materials to finding ways to incorporate them into customer applications to deliver breakthrough performance. Examples to illustrate these points will be shared in the presentations.

Plenary III

High Sectorially Resolved Inventories to Evaluate Air Quality Trends in China. SHU TAO, *Peking University*

Based on a set of high-sectorially resolved air pollutant emission inventories, impacts of socioeconomic transition and regulations on air pollution allevation in China were evaluated. Three case studies are presented to illustrate the lessons learned: 1) Impact of rural residential energy transition on air pollution and health; 2) Health effects of banning beehive coke ovens; and 3) Effectiveness of recent emission reduction efforts of major cities.

Rural household energy use is an important source of emission of air pollutants in China. However, the magnitude of rural household energy use, especially during the transition from use of solid fuels to clean fuels and electricity, has not been well quantified. To collect first-hand data on rural energy consumption and transition, the nationwide data were collected from a 34,489-household energy mix survey and a 1670-household fuel weighing campaign. It was found that the previous information from the International Energy Agency (IEA) and Food and Agriculture Organization (FAO) had significant errors. Consumption of wood and crop residue decreased by 61% and 57%, respectively, from 1992 to 2012 in rural China, much higher than the 15% and 8% reported by IEA and FAO. The fast energy transition that China is experiencing, primarily driven by an increase in income, has resulted in a significant emission reduction and health-climate co-benefit. It was estimated that the relative contribution of the rural residential sector to exposure to ambient PM2.5 decreased from 18±13 to 14±10 mg/m^3, that premature deaths decreased from 390 (360-420 as semi-quartile range) to 220 (200-250) thousand, and climate forces decreased from 0.057 ± 0.016 to 0.031 ± 0.008 W/m^2 during a period from 1992 to 2012, respectively. Still, the dependency of rural residents in northern China on traditional biomass and coal for heating is one of the most important factors contributing to ambient PM2.5 associated health outcomes.

Althoiugh beehive coke ovens, which was a major souce of benzo[a]pyrene, were banned by the Coal Law in 1996, they were not totally eliminated till 2011. The heath effects of historical beehive coke oven operation, the health benefits of the ban, and the adverse impacts of the poor implementation of the ban were quantitatively evaluated. Historical emissions of benzo[a]pyrene were re-constructed based on satellite images and used to model atmospheric transport, non-occupational population exposure, and induced lung cancer risk. It was demonstrated that more than 20% of the benzo[a]pyrene in ambient air was from beehive coke production in the peak production year. The cumulative non-occupational excess lung cancer cases associated with benzo[a]pyrene from beehive coke ovens was 3,500 (±1,500) from 1982 to 2015. If there was no ban, the cases would be as high as 9,290 (±4,300), indicating significant health benefits of the Coal Law. If the ban had been fully implemented immediately after the law was enforced in 1996, the cumulative cases would be 1,500 (±620), showing the importance of implementing the law.

Measures have been taken to reduce PM2.5 concentrations in China. However, the effectiveness of these measures has not been evaluated. To do so, confunding effects of meteorological factos have to be eliminated. A novel approach is applied to address this issue by individually quantifying the influences of emissions and meteorological effects on PM2.5 concentrations.Ambient PM2.5 concentrations from 1980 to 2014 were modeled subjected to three conditional scenarios that included a realistic situation, fixed emissions, and fixed meteorology. The differences among the model outputs were analyzed to quantify the relative contributions of emissions and meteorological factors. The output from the fixed-meteorology simulation was applied to develop regression models to predict emissions-driven PM2.5 concentrations, whereas the output from the fixed-emission simulation was adopted to establish probability functions to characterize the meteorological factor-induced PM2.5 fluctuations. The models were used to assess the effectiveness of the emissions reduction efforts implemented in major Chinese cities. It is demonstrated that the current decreasing PM2.5 trends in major Chinese cities are primarily driven by mitigation efforts, whereas the rebounds occasionally occurred due to the meteorological effects. Targeted emission reduction objectives of majority of cities have been exceeded so far. If the targeted emissions reduction goals can be fully achieved, the annual mean PM2.5 concentrations in 73% (55-89% as the 95% uncertainty interval) of the 190 major cities would reach the national standard of 35 μg/m^3 by 2030, and the percentage would be 94% (85-98%) if 50% extra efforts are made.

Plenary IV

Improvement of Inhalation Toxicity Testing for Nanomaterials and Compliance Monitoring for Ambient PM. Jun Kanno, Chuen-Jinn Tsai, *Japan Bioassay Res. C. Kanagawa; Natl. Chiao-Tung U., Taiwan*

For the new nanomaterials (NM), in general, there is no pre-existing knowledge to suggest its toxicity. Therefore, whole-body inhalation toxicity study is the first choice considering the most important route of exposure to humans. Yet, “inhalation” is a big hurdle for toxicologists; facilities are expensive to build and run, and requires skillful operators. Methods to generate well-dispersed aerosol and quantitate the aerosol density require case-by-case innovation, which is costly and time consuming. In order to overcome such hurdles, we developed the “Taquann” dispersion method and a “direct injection” whole body inhalation system. The dispersion method is based on two concepts: liquid-phase fine filtration and critical point drying to avoid re-aggregation by surface tension. Briefly, the bulk sample is suspended and dispersed in tert-butyl alcohol, filtered by a fine mesh to remove aggregates/agglomerates, snap-frozen by liquid nitrogen, and vacuumed, mimicking the process of critical point drying. Then aliquots of dry dispersed sample are periodically injected to the chamber system by the compressed air to maintain the aerosol concentration in the exposure chambers. This method is shown to be applicable to Mitsui-7 and Nikkiso MWCNTs, three different makes of nano-TiO_2, potassium titanate whiskers, and others. The advantages of this system is its cheapness and easy operation, high adjustability to various NM samples, low chance of polluting the facility, and low loss of sample. We believe our new system makes inhalation studies much popular to facilitate the risk assessment of not only various new NMs but also any other particulate matters including $PM_{2.5}$ from various origins.

While NM risk assessment is conducted *in vivo* or *in vitro*, most epidemiological studies link human health impacts to $PM_{2.5}$ mass measured at ambient environment. FRM $PM_{2.5}$ samplers and FEM monitors are used as compliance monitors, which make use of size-selective inlets followed by a filter to collect particles for further analysis. However, $PM_{2.5}$ concentrations determined by the FRM samplers are not true concentrations due to the uncertainties in the evaporation loss of volatile aerosol materials and water associated with aerosols during aerosol sampling and conditioning. The differences between $PM_{2.5}$ FEM and FRM concentrations often exist and increase with decreasing $PM_{2.5}$ concentrations. This talk will address the improvement in PM_{10} and $PM_{2.5}$ inlets, and aerosol conditioning during filter sampling which results in true $PM_{2.5}$ concentrations. The US EPA PM_{10} inlet and $PM_{2.5}$ inlet, including the well impactor ninety-six (WINS) and the very sharp cut cyclone (VSCC) were found to have particle bounce or particle overloading problems, which change the cutoff characteristics and PM concentrations. The grease-coated substrate of the PM_{10} inlet was replaced by an oil-soaked glass fiber filter to capture particles effectively. The impaction surface of the $PM_{2.5}$ WINS was re-designed to allow a small amount of water or vacuum oil to inject upward to wash deposited particles off the plate. The modified PM inlets eliminated particle bounce and particle overloading effectively with small errors during long-term sampling. A chilled filter sampler followed by a Nafion dryer was found to suppress the evaporation loss of semi-volatile inorganic materials (SVIM) effectively due to a small amount of water vapor condensation during sampling and conditioning processes. The total evaporation loss of SVIM in $PM_{2.5}$ measured by chilled filter sampler was effectively reduced and the accuracy of $PM_{2.5}$ sampling was significantly improved after correcting for the amount of condensed water determined empirically. These improvements lead to accurate PM data that can be related to health effects meaningfully and used to calibrate widely used low-cost PM sensors reliably.

Keywords: MWNT, nanomaterials, inhalation toxicity, aerosol sampling, PM inlet, $PM_{2.5}$.

Plenary V

On the Thermodynamics and Kinetics of Atmospheric Aerosol Formation. ILONA RIIPINEN, *Stockholm University*

The conversion of atmospheric vapors to aerosol particle and cloud hydrometeor populations depends on one hand on the energetics of the condensed phase, and on the other hand on the kinetics of the gas-phase molecules and particle populations. These thermodynamic and kinetic aspects are intertwined in aerosol formation processes, and generally difficult to isolate from field observations or even well specified laboratory data. Theoretically robust process models that accurately account for the kinetics and thermodynamics of aerosol formation are therefore critical for interpreting empirical data. The combination of such theoretical tools with experimental data on atmospherically relevant environments and molecules is the key for provide generalizable approaches to predict aerosol formation in e.g. climate and air quality models. In my presentation, I will summarize recent advances in understanding the key thermodynamic and kinetic features of aerosol formation, and discuss remaining key uncertainties in our efforts of creating approaches for describing aerosol formation with predictive power in various atmospherically relevant conditions.

1AC.1
Understanding Missing Sources of Fine Particulate Organosulfur Compounds in the Atmosphere: Implications from Ambient Measurements and Laboratory Experiments. MATTHIEU RIVA, Yuzhi Chen, Lindsay Yee, Hilary Green, Tianqu Cui, Nicole Olson, Nancy Ziying, Karsten Baumann, Mike Fort, Eric Edgerton, Eladio Knipping, Stephanie L. Shaw, Sri Hapsari Budisulistiorini, Caitlin Rose, Zhenfa Zhang, Avram Gold, Barbara Turpin, William Vizuete, Igor O. Ribeiro, Santos e Oliveira, Cristine Machado, Sérgio Duvoisin Junior, Rodrigo A. F. de Souza, Eliane Gomes, et al., *University of North Carolina at Chapel Hill*

Organosulfur compounds are ubiquitous in Earth's atmosphere. These compounds are non-negligible contributors to fine organic aerosol mass. Among them, sulfate esters or organosulfates (OSs) contribute the greatest mass fraction of particulate organosulfur compounds. These aerosol constituents are formed from multiphase chemical processes, such as the acid-catalyzed reactive uptake of gas-phase products generated from the atmospheric oxidation of biogenic and anthropogenic volatile organic compounds (VOCs) in the presence of aqueous sulfate aerosols. While the presence of OSs has been reported in fine aerosol collected from many locations, especially in biogenic-rich areas, the impacts of such products on the physicochemical properties of and the sulfate distribution within secondary organic aerosol (SOA) remain unclear. As sulfate over continental regions is generally of anthropogenic origin or from the oxidation of dimethyl sulfide, understanding the physical and chemical processes associated with SOA formation and properties, and how sulfate impacts them is crucial to properly representing SOA in models and evaluating their impacts on climate and human health.

SOA samples collected from the southeastern U.S. and the Amazon forest (isoprene and monoterpene-dominated atmospheres), were chemically characterized to evaluate the distribution of fine particulate organosulfur compounds. OSs and methanesulfonic acid (MSA) were quantified by ultra-performance liquid chromatography interfaced with electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (UPLC/ESI-HR-QTOFMS). Total organosulfur mass was determined by isotope ratio inductively coupled plasma mass spectrometry. OSs were found to contribute significantly to the organic aerosol (OA) mass in both areas. Total quantified OSs plus MSA, however, only accounted for about 50% of total organosulfur, suggesting the presence of a significant amount of unidentified organosulfur chemicals of different functionality, and unidentified processes that form them. We hypothesize that the missing mass is comprised of sulfate-containing oligomers formed from multiphase chemistry of BVOC oxidation products, especially the isomeric isoprene epoxydiols (IEPOX), with acidic sulfate aerosols. Targeted atmospheric simulation chamber experiments re-investigating the multiphase chemistry of IEPOX revealed that formation of OSs cannot fully account for the amount of sulfate consumed, suggesting that the missing source of organosulfur compounds can arise from previously uncharacterized IEPOX chemistry. Overall, our findings provide a comprehensive picture of particle-phase processing governing isoprene-derived SOA composition and suggest the role of IEPOX-OSs in SOA evolution has previously been underestimated.

1AC.2

Importance of Sulfate Radical Anion Formation and Chemistry in Heterogeneous OH Oxidation of Organosulfates. Kai Chung Kwong, Man Mei Chim, James F. Davies, Kevin Wilson, MAN NIN CHAN, *The Chinese University of Hong Kong*

Organosulfates are important organosulfur compounds present in atmospheric particles. While the abundance, composition, and formation mechanisms of organosulfates have been extensively investigated, it remains unclear how they evolve throughout their atmospheric lifetime. To acquire a fundamental understanding of how organosulfates chemically transform in the atmosphere, this work investigates the heterogeneous OH radical-initiated oxidation of sodium methyl sulfate droplets, the smallest organosulfate detected in atmospheric particles, using an aerosol flow tube reactor at a high relative humidity of 85 %. Aerosol mass spectra measured by a soft atmospheric pressure ionization source (Direct Analysis in Real Time, DART) coupled with a high-resolution mass spectrometer showed that neither functionalization nor fragmentation products are detected. Instead, the ion signal intensity of the bisulfate ion has been found to increase significantly after OH oxidation. We postulate that sodium methyl sulfate tends to fragment into a formaldehyde and a sulfate radical anion ($SO_4^{\bullet-}$) upon OH oxidation. The formaldehyde is likely partitioned back to the gas phase due to its high volatility. The sulfate radical anion can abstract a hydrogen atom from neighboring sodium methyl sulfate to form the bisulfate ion, contributing to the secondary chemistry. Overall, the heterogeneous OH oxidation of an organosulfate can lead to the formation of $SO_4^{\bullet-}$ and produce inorganic sulfate. Fragmentation processes and sulfate radical anion chemistry play a key role in determining the compositional evolution of sodium methyl sulfate during heterogeneous OH oxidation.

1AC.3

α-Hydroxy Organosulfates and Nitroxy Organosulfates Derived from Monoterpenes: Stability and Ambient Presence.

Yuchen Wang, Rongbiao Tong, JIAN ZHEN YU, *Hong Kong University of Science & Technology*

Organosulfates (OSs) derived from biogenic volatile organic compounds represent an important class of products formed between anthropogenic sulfur pollution and natural emissions. A lack of commercially available OS standards presents a significant obstacle to quantify this chemical interaction between human and nature. We synthesized α-hydroxy OS standards derived from eight monoterpenes (i.e., α- & β- pinene, limonene, sabinene, Δ3-carene, terpinolene, α-terpinene, and γ-terpinene) and two sesquiterpenes (i.e., α-humulene and β-caryophllene). After comparison of the MS/MS spectra and liquid chromatographic retention times between standards and ambient aerosol, we have positively identified α-hydroxy OSs derived from six monoterpenes (i.e., α- & β-pinene, limonene, sabinene, Δ3-carene, and terpinolene), and β-caryophllene in ambient samples from select locations in China, but failed to detect α-hydroxy OSs derived from α-terpinene, γ-terpinene, or α-humulene. With the exception of α-pinene, we did not detect OS regioisomers that have the sulfate group at the more substituted carbon position. This observation may have implication on OS formation mechanism, appearing to favor a diol intermediate pathway. Nitroxy organosulfates derived from limonene and β-pinene were also synthesized, providing opportunities to study their stability. Our work highlights the critical importance of having authentic standards in advancing our understanding of organosulfates.

1AC.4

Experimental Study of Condensed-Phase Reaction Kinetics of Secondary Organic Aerosols from Isoprene Expoxydiols.

YUZHI CHEN, Matthieu Riva, Theran P. Riedel, Havala Pye, Nicole Olson, Ziying Lei, Zhenfa Zhang, Avram Gold, William Vizuete, Barbara Turpin, Andrew Ault, Jason Surratt, *University of North Carolina at Chapel Hill*

Isoprene epoxydiols (IEPOX), OH-initiated oxidation products of isoprene, are known to produce secondary organic aerosol (SOA) through acid-catalyzed heterogeneous reactions in the presence of sulfate-containing aerosols within the atmosphere. IEPOX-derived SOA can contribute up to 40% of summertime organic aerosol mass in isoprene-rich regions like the southeastern U.S. Among all SOA tracers identified during laboratory and field studies, 2-methyltetrols and 2-methyltetrol sulfate esters, also referred to as IEPOX-derived organosulfates (OSs), together contribute a major mass fraction (e.g. >90% at Look Rock, TN) of IEPOX-derived SOA. Regulatory models that adopt rate constants for the formation of these two species from kinetic measurements in bulk solutions, however, typically yield discrepancies between model predictions and observations suggesting a need for more accurate reaction-rate constants with sulfate-containing aerosols. Non-ideality of aerosols may affect the applicability of kinetic measurements from bulk solution studies. While computational estimates of the reaction-rate constants that took into account the non-ideality of aerosols were, on average, 2-3 orders of magnitude higher than those derived from measurements in bulk solutions (especially for IEPOX-derived OSs), and seemed promising to improve the model representation of IEPOX uptake process, supporting laboratory measurements are still lacking. We have developed an alternative approach that couples chamber experiments with offline chemical characterization and modeling to derive condensed-phase reaction-rate constants in IEPOX-derived SOA. These previous experiments, however, were conducted under only dry conditions (RH <5%) limiting our ability to extend the derived reaction-rate constants to more humid conditions. In addition, the lack of time-resolved reaction profiles of 2-methyltetrols and IEPOX-derived OSs and the potential for artifacts induced by filter collection also introduce uncertainties in the reaction-rate constants derived from the previous study.

In this work, chamber experiments were conducted using gaseous IEPOX and acidic sulfate aerosols to generate IEPOX-derived SOA in the UNC indoor chamber facility. Chamber-generated IEPOX-derived SOA samples were collected by a particle-into-liquid sampler (PILS) using a 5-minute time resolution. PILS samples were immediately analyzed by ion chromatography (IC) for inorganic constituents and ultra-performance liquid chromatography interfaced to high-resolution quadrupole time-of-flight mass spectrometry equipped with electrospray ionization (UPLC/ESI-HR-QTOFMS) for IEPOX-derived SOA tracers. Our results show that up to 90% of the inorganic sulfate was converted to IEPOX-derived OSs and oligomers in acidified ammonium sulfate particles within one hour of reaction with gas-phase IEPOX. Our results further demonstrate that the rates of IEPOX-derived OS formation were likely underestimated by prior bulk-solution kinetic studies. New condensed-phase reaction-rate constants for the formation of the 2-methyltetrols and IEPOX-derived OSs were derived from a one-dimensional box model of our chamber experiments using characterized reaction profiles resolved by PILS-IC and PILS-UPLC/ESI-HR-QTOFMS. The impacts of new reaction-rate constants on aerosol acidity and atmospheric formation of IEPOX-derived SOA need to be further assessed with updated air quality and global models, which is critical in understanding the governing processes that lead to SOA formation and developing air-pollution mitigation strategies.

1AC.5

Photochemical Multiphase Organonitrate Formation in Wet Particles Under Humid NOx Conditions. YONG LIM, Jihoon Seo, Jin Young Kim, Bong Kim, Barbara Turpin, *KIST*

NOx plays an important role in urban atmospheric chemistry. NOx, which is emitted from the fossil fuel combustion, affects secondary aerosol formation. Traditionally, NOx is known to be associated with gas-phase reactions forming semi-volatile products like organonitrates or ammonium nitrates, leading to secondary aerosol. Here, we discover organonitrate formation in the aqueous phase. We have conducted chamber experiments for photooxidation of wet aerosols containing glyoxal and ammonium sulfates under humid NOx conditions, and analyzed the products using high resolution quadrupole time of flight mass spectrometry (HR-Q-TOF-MS) and a scanning mobility particle sizer (SMPS). Nitric acid is dominantly formed by photooxidation of NOx and taken up into neutral wet particles substantially, resulting in dramatic hygroscopic growth at high relative humidity. In turn, increased aerosol liquid water in wet particles facilitates aqueous-phase reactions of glyoxal and dissolved nitric acid leading to organonitrate formation. We have identified several types of organonitrates formed by the reaction of glyoxal and nitric acid in the aqueous phase. We have also conducted the quantitative analysis for organonitrates by preparing standard solutions of glyoxal, nitric acid, and organonitrates from glyoxal-nitric acid mixtures with known concentrations. Using a thermodynamic model and a kinetic/equilibrium model based on smog chamber results, we have simulated ambient particle components (particularly, nitrates, organics and organonitrates) and particle acidity during the haze event at Seoul, the most urbanized city in South Korea, which is characterized by high NOx and relative humidity. HNO3 uptake into the particles and the hygroscopic growth and acidification of the particles were significant, and notably organonitrates were formed significantly. Our finding of organonitrate formation in the aqueous phase provides a new insight of secondary organic aerosol, enhancing our understanding and model predictions for organic particles, whose formation is still not well explored.

1AC.6

Quantifying the Hydrolysis Rate of Daytime and Nighttime Organic Nitrates in Aerosol Water. MASAYUKI TAKEUCHI, Thomas Berkemeier, Gamze Eris, Nga Lee Ng, *Georgia Institute of Technology*

Ambient field studies have observed a varying level of atmospheric gaseous and particulate organic nitrates across different continents and many found that their contribution to fine organic aerosol mass is substantial. Depending on the fate, these organic nitrates could act as a reservoir and/or permanent sink of reactive oxidized nitrogen species (i.e. NO_x), which eventually determines the production potential of tropospheric ozone. Modeling results using recent field measurement data in the Southeastern U.S. suggest that the lifetime of submicron particulate organic nitrates is on the order of several hours, though the loss mechanism is not known. Due to their direct impact on the NO_x cycling, ozone and secondary organic aerosol (SOA) formation, it is crucial to understand the dominant loss mechanisms of organic nitrates in the atmosphere and parameters that affect the loss rate. Among various loss mechanisms, particle-phase hydrolysis is a known loss mechanism of particulate organic nitrates in the presence of aerosol water and is generally considered a major loss process. However, studies quantifying the hydrolysis rate of particulate organic nitrates are currently scarce, in part due to the difficulty of isolating the effect of hydrolysis from other confounding processes, such as potential RH-dependent loss of organic nitrate vapors to Teflon chamber walls. Here, our study aims at quantifying the hydrolysis rate of particulate organic nitrates from α-pinene and β-pinene under two oxidation conditions: photooxidation in the presence of NO_x (i.e. daytime) and NO_3 oxidation (i.e. nighttime), taking into account the difference in organic nitrate vapor wall loss rate at different RH. Experiments are conducted in the Georgia Tech Environmental Chamber (GTEC) facility. A large suit of oxidized, speciated gaseous and particulate organic nitrates are measured by Filter Inlet for Gases and AEROsols coupled to High-Resolution Time-of-Flight Chemical Ionization Mass Spectrometer (FIGAERO-HR-ToF-CIMS). The total gaseous and particulate organic nitrates are monitored by Thermal-Dissociation Cavity Attenuated Phase Shift Spectrometer (TD-CAPS), and the total particulate organic nitrate concentration is estimated by High-Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS). For the photooxidation win the presence of NO, there was a clear trend in the evolution of speciated particulate organic nitrates that $C_{10}H_{17}NO_x$ (x = 5-8) peaked first suggesting the first generation products, followed by the peaks of $C_{10}H_{15}NO_x$ and $C_{10}H_{13}NO_x$ indicating further OH aging to produce compounds with lower H:C and higher O:C ratios. This process is expected to take place by the abstraction of H, reaction with NO to create an alkoxy radical, which then forms a carbonyl via decomposition. However, regardless of the molecular formula, all speciated C_{10} particulate organic nitrates, when normalized humid to dry experiments, follow a similar decreasing trend that is identical to the bulk behavior observed in HR-ToF-AMS. This could indicate that the first oxidation step is more important than later steps in determining the susceptibility of particulate organic nitrates. Additionally, we experimentally determine the wall loss rate of organic nitrate vapors in our chamber facility under dry and humid conditions. Results from applying the experimental values in the aerosol kinetic model will be presented and the impact of organic nitrate vapor wall loss on the quantification of hydrolysis rate will be discussed.

1AC.7

Impact of NOx on Secondary Organic Aerosol (SOA) Formation from α-pinene and β-pinene Photo-Oxidation: The Role of Organic Nitrates. Iida Pullinen, SEBASTIAN H. SCHMITT, Mehrnaz Sarrafzadeh, Sungah Kang, Patrick Schlag, Stefanie Andres, Einhard Kleist, Thomas F. Mentel, Franz Rohrer, Monika Springer, Ralf Tillmann, Jürgen Wildt, Cheng Wu, Defeng Zhao, Andreas Wahner, Astrid Kiendler-Scharr, *Forschungszentrum Jülich*

Impacts of nitrogen oxides (NO_X) on the formation of gas phase organic nitrates (ON) and subsequent Secondary Organic Aerosol (SOA) mass formation were investigated in a constantly stirred tank reactor. This work focuses on understanding the mechanisms that results in suppression of SOA mass formation from α-pinene and β-pinene photo-oxidation in the presence of high NO_x concentrations. Here we will demonstrate that ON formation alone cannot explain this NOx impact.

Effective uptake coefficients (γ_{eff}) were measured for Highly Oxidized Multifunctional molecules (HOM), which has been found to be dependent on the number of oxygen atoms in the respective HOM. It has been observed that HOM with more than 6 O-atoms were efficiently lost on particles while the loss of HOM containing more than 8 O-atoms, was collision limited. There was no systematic difference between γeff measured for HOM-organic nitrates (HOM-ON) and other monomer termination products such as ketones, alcohols or hydroperoxides. This similarity was attributed to the multifunctional character of the HOM. Since both number and character of most functional groups in monomer HOM with the same precursor HOM-peroxy radical are identical, the vapor pressures of such HOM are within the same range. Thus the suppressing effect of NO_X on SOA formation cannot be explained by the production of HOM-ON replacing other monomer termination products of peroxy radical – peroxy radical reactions.

Comparison of the fraction of organic bound nitrate ($OrgNO_3$) stored in potential particle precursors to the fraction of $_{OrgNO3}$ in the particles, revealed a substantial lack of $OrgNO_3$ in the particle phase. This suggests a strong sink for organic nitrates in the particles. This sink could be due to hydrolysis which forms either HNO_3 or an organic rest. Evaporation of HNO_3 formed by hydrolysis of HOM-ON could possibly explain the missing OrgNO3 in the particle phase but not the 20-30 % lower SOA yields in presence of high NO_X concentrations.

1AC.8

The Impact of Aerosol Uptake of Organic Nitrates on Simulated Surface Ozone in CAM-Chem. REBECCA SCHWANTES, Louisa Emmons, Simone Tilmes, John Orlando, Geoffrey Tyndall, *National Center for Atmospheric Research*

Many regions in the United States have poor air quality because of high levels of ozone. Ozone is intrinsically hard to simulate in global and regional models because the amount of ozone present is controlled by large non-linear sources and sinks. Recently, the chemical mechanism for isoprene and monoterpene oxidation has been updated in CAM-Chem (Community Atmosphere Model with chemistry), which is a component of the Community Earth System Model (CESM). Assumptions made in the model about the aerosol uptake of organic nitrates derived from isoprene and monoterpene oxidation significantly impact ozone formation. This study will comprehensively examine assumptions made in the aerosol uptake of various organic nitrates in the model including those derived from isoprene and monoterpene oxidation. Additionally, if necessary, the aerosol uptake of other relevant chemical compounds will also be updated. The updated model results will be evaluated against data collected during the Studies of Emissions Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys (SEAC4RS) field campaign. The impact of uncertainties in the organic nitrate aerosol uptake on simulated surface ozone will be presented to motivate and direct future research in understanding this complex process. Results suggest that a more explicit treatment of secondary organic aerosol formation in models used to understand air quality is not only necessary for describing aerosol correctly, but also necessary for accurately simulating ozone.

1AM.1

Insights into Isoprene-Epoxydiol SOA Chemistry in Cloud Droplets using WRF-Chem and HI-SCALE Field Observations.

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Multiphase chemistry of isoprene epoxydiols (IEPOX) is an important pathway resulting in the formation of IEPOX-SOA. A number of studies report substantial IEPOX-SOA formation on wet sulfate aerosols, at many locations globally. However, IEPOX-SOA formation in clouds has not been reported previously. Measurements during recent HI-SCALE field Campaign provide direct evidence for IEPOX-SOA formation in cloud droplets.

To simulate this process, we implemented IEPOX-SOA chemistry module in WRF-Chem and applied this chemistry to both wet interstitial aerosols and cloud droplets based on the simpleGamma multiphase kinetic model [Woo and McNeill, 2015]. WRF-Chem simulations are conducted at high spatial resolution (1.3 km grids). We analyze model results over the southeast part of our modeling domain that abounds in biogenic isoprene emissions. Simulations show that at cloud level, average concentration of gas-phase IEPOX that dissolves in cloud droplets (40 ng m-3) is an order of magnitude higher compared to dissolved IEPOX in wet aerosols (3 ng m-3) due to significantly larger cloud droplet water content as compared to interstitial aerosols. Further reaction of dissolved IEPOX results in the formation of IEPOX-SOA. However, since reaction kinetics are significantly slower in more dilute cloud droplets as compared to interstitial aerosols, previous studies often neglect the role of cloud chemistry in IEPOX-SOA formation. In contrast, our simulations indicate that formation of IEPOX-SOA in clouds is 3 times greater than IEPOX-SOA in interstitial aerosols. Simulations indicate that conversion of dissolved IEPOX to IEPOX-SOA is indeed slower in cloud droplets compared to interstitial aerosols (10% in cloud droplets, 50% in interstitial aerosols). However, this slow conversion is compensated by large amounts of dissolved IEPOX available in cloud droplets compared to interstitial aerosols. Model results are in good agreement with measurements by the single particle mass spectrometer, miniSPLAT, which indicates preferential formation of IEPOX-SOA in cloud droplets. Simulations also indicate that when cloud droplets evaporate, cloud-phase IEPOX-SOA becomes part of interstitial aerosols, increasing interstitial IEPOX-SOA by a factor of 2. Future work will investigate factors affecting observed regional variations in IEPOX-SOA such as variations in aerosol and cloud properties, biogenic emissions, and their aging in the atmosphere.

1AM.2

Long-term Trends in Simulated Ultrafine Particle Concentrations in California. Xin Yu, Anikender Kumar, Melissa Venecek, Abhishek Dhiman, MICHAEL KLEEMAN, *University of California, Davis*

Ambient ultrafine particles have toxic properties due to their high ratio of surface area to volume that promotes biochemical reactions with adsorbed components such as metals. Ultrafine particles can also cross cell membranes once inside the body allowing them to reach a wide range of organs. Recent epidemiological studies have shown that ultrafine particles are associated with premature death in California, but comprehensive exposure data for ultrafine particles are missing which makes it difficult to estimate the total public health impact.

Here we predict exposure fields for ultrafine particles over California for the period 1996 through 2016 with 4km spatial resolution and daily time resolution. Long term trends in ultrafine particle concentrations are compared to field measurements that span this study period. Source apportionment predictions based on the regional model calculations are compared to receptor-oriented source apportionment results using the chemical mass balance (CMB) model and the positive matrix factorization (PMF) model. The effects of various control programs for mobile sources and biomass combustion are investigated in both the modeled concentrations and the measured concentrations of ultrafine particles over the decades. Implications for exposure and public health are discussed.

1AM.3

Physical and Model-based Characterization of NPF Events and Sensitivity of CN and CCN to Changes in Anthropogenic Emissions in the Midwestern United States. Can Dong, Robert Bullard, Ashish Singh, Scott N. Spak, Hitoshi Matsui, CHARLES STANIER, *University of Iowa*

New particle formation (NPF) is a frequently observed phenomenon worldwide. Ten months (July 2013 to June 2014) of continuous measurements of particle number size distribution were performed at a rural Midwestern United States location (Bondville, Illinois), spanning sizes from 3 nm to 2.5 microns. Bondville is representative of Midwestern United States and other perturbed continental locations with moderate sulfur dioxide (SO2) and fine particulate matter (PM2.5) concentrations (i.e. SO2 of 0.5-3 ppb, PM2.5 of 5-15 µg/m3) at background sites.

New particle formation behavior at the site is similar to other mid-latitude sites, with NPF in 2013-2014 occurring on 44.1% of classifiable days, highest NPF frequency in spring and fall, followed by summer and lowest in winter. Observed growth rates for measured nucleation mode particles (3-25 nm) were highest (8.97 nm/h) in summer and lowest (1.45 nm/h) in winter.

SO2 and sulfate concentrations are dropping in the region, and the fractional importance of secondary organic aerosol is increasing (SOA). For example, at Bondville, SO2 fell from 2.1 to 0.8 ppb from 2005 to 2013, a 62% decrease. As a test of the nucleation explicit version of WRF-Chem, which simulates nucleation using a 20-bin sectional model down to 1 nm, each season was simulated using 2005 NEI (higher SO2 emissions), 2011 NEI (lower SO2 emissions), and sensitivity tests were done with inclusion and exclusion of growth by SOA.

NPF events were captured well by the NPF-explicit WRF-Chem model in April and November without considering secondary organic aerosol (SOA) formation. The two anthropogenic emission inventories, i.e. 2005 NEI and 2011 NEI, were used to study sensitivities of CN (condensation nuclei) and CCN (cloud condensation nuclei) to emissions in the Midwest. Modeling results show that SO2 emission reduction is the primary cause for CN number concentration change. Switching SO2 emissions from 2005 NEI to 2011 NEI led to significant decrease of CN10 (particles with sizes larger than 10 nm) number concentrations, especially in April, September and November (over 20% decrease). On average, model simulated SO2 concentrations by using 2011 NEI were approximately half of the values simulated by using 2005 NEI (2.17 ppb vs 4.32 ppb). Changes of primary aerosol and NH3 emissions also play a role, but the influence is not as significant as that of SO2. Simulated changes of CCN at lower water supersaturations (0.2%) were complicated due to interactions between meteorology and chemistry. At higher water supersaturations (1%), CCN changes were consistent with that of CN10.

Comparison to independent measurements of ultrafine particle number with height (by numerous light aircraft flights) showed that the model's aerosol number predictions do not decrease fast enough with height, an indication of the model having too much vertical mixing, insufficient particle removal, or too strong of a free tropospheric nucleation source.

During the February and September simulation periods, bursts of new particles were reproduced but the subsequent growth was not. The sensitivity of model performance on meteorology and SOA is discussed. Finally, simulations with very low SO2 emissions are performed to show the impacts on air quality, CCN, and the number size distribution under future such scenarios.

1AM.4

Mutual Information Method for Understanding Key Variables in Atmospheric New-Particle Formation. MARTHA ARBAYANI ZAIDAN, Ville Haapasilta, Rishi Relan, Pauli Paasonen, Veli-Matti Kerminen, Heikki Junninen, Markku Kulmala, Adam S. Foster, *Helsinki University*

New-particle formation (NPF) is an important phenomenon occurring in the atmosphere. This process is very non-linear and complex, involving atmospheric chemistry of precursors and clustering physics as well as subsequent growth before NPF can be observed. Thanks to ongoing efforts, tremendous amounts of atmospheric data is now available, generated from simulation models and laboratory experiments as well as continuous measurements directly from the atmosphere. This fact makes data analysis by human brains as well as via traditional statistical methods more challenging, but on the other hand enables to usage of modern data science techniques. In this work, we investigate the use of mutual information method to understand the relationship between observed NPF events (measured at Hyytiälä, Finland) and a wide variety of simultaneously monitored ambient variables: trace gas, aerosol particle concentrations, meteorology, radiation and a few derived quantities. The investigation aims to identify key factors contributing to the NPF. The applied mutual information method finds that the formation events correlate with water content, sulfuric acid concentration, ultraviolet radiation, condensation sink and temperature. Previously, these quantities have been known to be key factors in the phenomenon via dedicated field studies and laboratory as well as theoretical research. The novelty of this work is in demonstrating that the same results can be obtained by the proposed data analysis method which operates without supervision and physical insight. This suggests that the method is appropriate to be implemented widely in the field of atmospheric sciences to discover other interesting phenomena and its relevant variables.

1AM.5

Efficient Wet Removal of Soluble Species through Deep Convection Simulated in Chemistry-Climate Models. PENGFEI YU, Karl D. Froyd, Owen Toon, Charles Bardeen, Shang Liu, Ru-Shan Gao, Christina Williamson, Agnieszka Kupc, Charles Brock, Joshua P. Schwarz, Michael Mills, Simone Tilmes, Karen Rosenlof, Daniel Murphy, *NOAA ESRL and CIRES*

Convective transport determines the vertical transport efficiencies of aerosols and other trace gases in the chemistry-climate models. Parameterizations of convective transport in numerical models especially in chemistry-climate models are of large uncertainties. In the study we shows that the default parameterization scheme in NCAR/DOE Community Earth System model shows a large discrepancy of a factor of 10-1000 on aerosol mass budget against the observations. A modified transport scheme considering activation of aerosol above cloud-base and aerosol-cloud interactions in the sub-grid scale provides much improved agreements. We use various measurements on aerosol mass concentration from a number of field campaigns including Atom1, HIPPO1-5, and balloon-borne measurements over Kunming, China to validate and quantify the convective transport efficiency in chemistry-climate models.

1AM.6

New Method to Modeling Heterogeneous Reaction of SO2 during Haze in China. SHUPING ZHANG, Jia Xing, Biwu Chu, Hong He, Golam Sarwar, Kebin He, Yan Zhao, *RCEES, CAS, China*

In recent years, haze in China has been a hot topic in the study of aerosol chemistry and modeling, while the simulation of heterogeneous sulfate formation is still a big challenge. Literature suggests that different studies used different parameterized methods and heterogeneous oxidation rate of SO_2, which limits application of the haze modeling. To address that issue, this study developed a parameterization using experimental results that are more direct and approximate to the haze generation conditions in China, based on the linear interpolation of the literature uptake coefficient. After summarizing the relevant coefficient of uptake, a series of experiments are conducted to investigate the heterogeneous uptake of SO_2 under the atmospheric reaction condition of different relative humidity with the coexistence of NH_3 and NO_2 on the real dust surface. The uptake coefficient under different relative humidity in CMAQ model is parameterized based on the experimental results. We establish a parametric approach to model the heterogeneous oxidation of SO_2 to sulfate under the coexistence of NH_3 using the more direct experimental data. This parameterization method can improve the model performance in the simulation of Beijing sulfate in winter 2014 by 9.18%. The heterogeneous oxidation of SO_2 in the presence of NH3 can contribute to 17% of the sulfate concentration during periods of heavy pollution.

1AM.7

Sparse-particle Methods for Simulation of Atmospheric Aerosol. LAURA FIERCE, Robert McGraw, *Brookhaven National Laboratory*

Aerosol effects on clouds and radiation have remained a large source of uncertainty in quantifying anthropogenic changes to the Earth's energy balance, despite increases in model complexity. Climate-relevant aerosol properties depend on characteristics of individual particles, but particle-level characteristics are not easily represented in global models. Instead, global and regional aerosol schemes approximate the representation of particle size and composition, leading to errors in prediction of direct and indirect aerosol effects that have not been well quantified. At the other extreme, the particle-resolved PartMC-MOSAIC simulates the evolution of the full particle mixing state using a Monte Carlo approach but is computationally too expensive for large-scale simulation. Here a new framework is introduced for simulation complex aerosol distributions, based on the quadrature method of moments. Key features of aerosol populations are captured using quadrature approximations of multivariate moments. Each quadrature consists of a collection of abscissas, or representative particles, and associated weights. Distributions with respect to key aerosol quantities, such as the critical supersaturation for CCN activation or optical cross sections, can be approximately reconstructed using constrained maximum entropy distributions. Unlike other reduced aerosol schemes, such as modal and sectional models, the sparse-particle approach is not constrained to pre-determined size bins or assumed distribution shapes. CCN activity and optical properties from the sparse aerosol simulations are benchmarked against the particle-resolved model PartMC-MOSAIC. This study is a first step toward a new aerosol simulation scheme for large-scale simulations that will track multivariate aerosol distributions with sufficient computational efficiency for large-scale simulations.

1AM.8

Constraining Aerosol Processes with a Stability-Based Inverse Model. DANA MCGUFFIN, Peter Adams, Erik B. Ydstie, *Carnegie Mellon University*

The general dynamic equation predicts the evolution of aerosol size distributions with terms that represent emission, nucleation, condensation, coagulation, and deposition of particles. This work aims to constrain key uncertain terms in the general dynamic equation using measured size distributions. Coagulation of particles is calculated based on their Brownian motion and the loss rate includes deposition to the ground and advection. However emission, nucleation, and condensation of volatile organic compounds (VOCs) are highly uncertain. Primary aerosol emissions are difficult to monitor and calculate due to the variability in emission fluxes and intensity levels within a sector. The nucleation of particles from molecular clusters of compounds possibly including sulfuric acid, water, amines, and organic compounds is still an active area of research. Secondary organic aerosols (SOA) are generated as VOCs condense to the particle phase or on pre-existing aerosol, but there are large uncertainties in the identity of VOC precursors and the condensation mechanism as well as in the SOA budget.

The goal of this work is to use measured aerosol size distributions to gain knowledge on three uncertain aerosol processes: primary organic aerosol emissions, nucleation rate, and SOA production. Such measurements of aerosol mass and number size distributions implicitly contain a great deal of information about these microphysical processes, and they are available at several ground sites. We integrate size distribution measurements and an aerosol microphysics model using nonlinear process control theory.

Measured size distributions are generally used to validate models through sensitivity analyses in forward models. In these cases, tuning factors or model parameters are systematically adjusted until the model reproduces a measured distribution of aerosols. However, a more robust way to do this is to generate and run an inverse model.

In general, inverse models are used to constrain uncertain processes based on a set of measurements. Inverse models usually minimize a cost function related to the sum of squared error in the set of observations by linearizing the forward model. However, inverse modeling of aerosol microphysics is challenging since it involves nonlinearities that span large spatial and temporal scales. This work develops a new, stability-based inverse modeling technique that is not computationally intensive and rigorously accounts for nonlinear dynamics.

Here, we present the development of the inverse modeling technique and preliminary applications to a box model. We use a zero-dimensional version of the TOMAS microphysical code, which models size-resolved aerosols with the discretized general dynamic equation. We generate synthetic measurements by running TOMAS with a set of “true” rates for primary emissions, nucleation, and SOA production. Then, we start a TOMAS simulation with a set of process rates biased from their “true” value. We will see if the developed inverse modelling technique will estimate the “true” process rates based on the synthetic measurements. The methodology developed here will facilitate future work that estimates primary aerosol emissions, nucleation, and SOA production in a global model based on a measurement network.

1CM.1

Comparison of Different Neutralizing Methods by IPA on Electret Filter Media. MIN TANG, Sheng-Chieh Chen, Drew Thompson, David Y. H. Pui, *University of Minnesota*

It has been broadly demonstrated that electrostatic charges added to polymer fibers by creating electrets will improve particle capture abilities without increasing the pressure drop. Filtration applications require knowledge of the minimum efficiency provided by a filter (worst-case performance). In existing test standards, e.g. EN 779 and ISO 16890, isopropanol (IPA, in liquid or vapor phase) is used to eliminate electrostatic effects from filter media. There is few report about whether IPA liquid and vapor can fully discharge the electret media. Currently, there is a huge controversy in fiber charge characterization techniques for electret media. This study developed a simple and reliable method to determine whether the filter media were fully discharged. The neutralization effect of IPA liquid and vapor discharging was compared. The results showed that IPA vapor treatment showed better neutralization effect than IPA liquid immersion, since IPA liquid treatment can induce undesirable charges on fiber surface. It was found that IPA vapor did not have the ability to discharge electret media. The discharging process was that IPA vapor condensed on the charged surface and remove the static charge. Proper design of IPA vapor chamber to allow vapor condensation on fiber surface is important to efficiently remove charges of electret media.

1CM.2

Filtrationof Liquid Aerosol on Fibrous Filters Modified with Silica Aerogel - Experimental and Modeling Study. JAKUB GAC, Bartosz Nowak, Marta Bojarska, *Warsaw University of Technology*

Removal of liquid droplets from gas flow is one of the most important process in many industrial processes (i.e. gas processing) environmental protection (air cleaning). One of the most efficient method to manage it is a filtration of a fibrous filters. For a last decade some methods of additional improvement filtration efficiency on such filters are investigated.

In our work we propose the modification of filters by covering their fiber with silica aerogels. These aerogels are material characterised by very high porosity, low density and extremely oleofilic properties. In our study they are obtained by means of sol-gel process. Last stage of this process is conducted in the presence of fibrous filter what causes the deposition of aerogel on fibers of this filter.

Our investigations show that such a filter has much greater efficiency than unmodified one. One of the reason us a presence of aerogel structures which act as additive collectors. The other effect is good sorprive properties of aerogel in respect to oil.

The experimental findings are confirmed with results of modeling of oil droplet filtration of single fiber covered by aerogel structure.

1CM.3

Adsorption Characteristics of Sub-10nm Nanoparticles on Porous Materials. ZIYI LI, Yingshu Liu, Chuen-Jinn Tsai, Yi Xing, Pei Lu, Likun Yin, Ralph Yang, *University of Science and Technology Beijing*

Adsorption of tiny nanoparticles with sizes close to gases on porous materials, such as activated carbons and zeolites, has been a long-existed and unrevealed issue in the gas separation field. Several recent studies dealing with PM2.5 using activated carbons (Kim et al., 2016), MOFs-coated filters (Chen et al., 2017), and nanofiber-coated window screens (Khalid et al., 2017) have shown functions of porous structure in trapping particles, and thus the lack of consideration on filter material effects for predicting filtration efficiency at nanometer range based on traditional theory. On the other hand, nanoparticles behaving like gas molecules are able to easily diffuse deep into porous networks, which would influence the utilization of adsorbents in practical gas separation (Kim et al., 2017), and needs theoretical directions for protection.

Herein, we demonstrate this particular phenomenon by conducting the removal efficiency test for sub-10 nanoparticles filtered by mesoporous adsorbents with different morphologies, including CMK-3, CMK-5, KIT-6, and a series of SBA-15 with the primary pore size range of 5.8-17.8 nm, and by FAU zeolites ion-exchanged with different cations such as Li+, Na+, K+, Mg2+, Ca2+ and Sr2+. The results show efficiency curves different from those predicted by Brownian diffusion filtration theory which always get close to 100% below 10nm, and varied in a regular manner with adsorbent properties. The effects of morphologies, pore size distributions and ion exchange properties on nanoparticle capture will be explored in details based on material characterizations, adsorption theories, and molecular simulations.

Keywords: nanoparticles, porous materials, adsorption, removal efficiency test, molecular simulation

Reference:

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1CM.4

Filtration Performance of a Melt Electrospun Filter Material. DAINIUS MARTUZEVICIUS, Dalia Buivydiene, Edvinas Krugly, Darius Ciuzas, Tadas Prasauskas, Linas Kliucininkas, *Kaunas University of Technology, Lithuania*

INTRODUCTION. Air filtration sector continuously seeks of the development of high-durability filters, having high efficiency and low pressure drop. Nanofbrous filters, however, face issues with relatively low quality factor, since high efficiency is counter levered by high pressure drop. Melt electrospinning has emerged as an efficient technique for the formation of polymer nonwowen filtration mats. Such technique may be tuned so that the produced fibres range broadly in diameter, providing optimum efficiency with relatively low pressure drop. The presented study presents the development and testing of such filtration media.

METHODS AND MATERIALS. The prototype fibre printing apparatus was constructed by uniting principles of additive 3D printing and melt electrospinning. The apparatus consisted of movable arm holding electric heater and exchangeable nozzles combined with high voltage source to form a positively charged electrode. A spinning collector drum served as a grounded electrode.

A commercially available polymer having a relatively low viscosity and high melt flow rate (Vestamid™ L 1600, Evonik AG) was spun. During 1 hour of spinning, a mat of the area 150 cm2 with mass, depending on feed rate of polymer ranging from 26 g/m^2 to 122 g/m^2.

The obtained fibre mats were subjected to the air filtration tests. NaCl aerosol was generated using Collison nebulizer (Model CN 24 J, BGI Inc., USA), dried by diffusion dryer packed with silica gel, diluted with dry air and charge equalized using bi-polar neutralizer (3054A, TSI Inc.). 37 mm round sample of mats were tested, measuring upstream and downstream concentrations of particles by ELPI+ (Electrical Low Pressure Impactor, Dekati Ltd., Finland). The pressure drop before and after filtration media was measured by a pressure sensor (Model P300-5-in-D, Pace Scientific Inc., USA). Filtration efficiency (η) and Quality Factor (QF) were calculated based on the particle concentration measurements.

RESULTS. Various distributions of fibre diameters were obtained, with the mean ranging from 2.8 to 8.6 µm. By-layered structure has been achieved, with the top layer slightly more uniform with diameter modes at ≤1 µm and between 2 - 5 µm while bottom layer was a mixture of fibres with diameters ranging from 0.3 to 27.4 µm distributed in bi- or three modal manner.

The quality factor was calculated as a ratio between filtration efficiency and pressure drop with the aim to better compare manufactured filter media to off-shelf filtration materials. The calculated quality factor ranged from 0.206 Pa^{-1} to 0.320 Pa^{-1} for different mats. As a comparison, the tested commercial H13 filter material had a QF of 0.029 Pa^{-1}. Such higher performance of the melt-spun materials may be attributed to an optimum morphology as well as lower base weight.

Further challenges to the optimization of the setup include increasing through output of the spinning. A polymer material having decreased melting temperature and increased melt flowrate as well as bearing high mechanical stability would also increase the opportunity for the expansion for this technique in air filtration sector.

1CM.5

Filtration Performances Study of Porous Media Composing Protective Clothing Against Solid Aerosols. LOÏC WINGERT, Ludovic Tuduri, Yves Cloutier, Stéphane Hallé, Ali Bahloul, Dominique Tessier, Jean-Luc Giraudel, Patricia Dolez, Pearl Yip, *IRSST/ETS*

Aerosols found in workplaces depend on workers activity or industrial processes (metallization, asbestos removal or waste treatment …). The particles emitted by these activities can be very different from each other. Metallization fumes are made, for example, of ultrafine particles (UFPs) of metal oxide whereas those found in electronic waste industry are often micron-sized and composed of heavy metals. Some micron-sized particles, such as the beryllium, represent a proven health hazard by skin contact leading to airborne dermatitis. Only a few studies are available on skin damages related to UFPs. Nonetheless, they already highlight a risk of cytotoxicity and migration to ganglia and organs. Despite these potential danger to the skin, no cutaneous threshold limit values (TLV) exists for solid aerosols. This absence of TLV together with the known health hazards of some common solid aerosols and the lack of knowledge on the UFPs has led, as a precaution, to the use of chemical protective garments (CPG). According to the ISO 16602 standards, CPG against solid aerosols are classified as type-5 and must meet a minimal performance level defined by the ISO 13982-1 and ISO 13982-2 standards. Since there is no hierarchy between all the certified type-5 CPG, significant differences between their protective efficiency could exist and this might lead to an over or under-protection of the workers.

Thus, it was decided to study the filtration performances of the fabrics/materials composing a wide range (20) of type-5 CPG among those available in North America. Amongst, the CPG selected for this study nine were made of microporous fabrics (MP), ten of multilayered nonwoven fibrous media (SMS, SMMS/SMMMS)* and one of a fabric produced by flash spinning process (FS). In order to expose these materials to a wide range of particle sizes (ultrafine to micron-sized), such as those that could be found in workplaces, a 20 nm to 2000 nm diameter sodium chloride aerosols was produced by nebulization in a wind tunnel. Furthermore, penetration experiments were performed at three different low air velocities (0.05, 0.15, 0.3 cm/s) in order to be as close as possible to velocities encountered in real situations. To ensure the robustness of the results, each experiment was triplicated. The collection efficiency was computed from the particle size distributions measured upstream and downstream of the tested samples by using a SMPS (3936, TSI) / APS (UVAPS 3314, TSI) tandem. In addition to the penetration or collection efficiency, the air permeability of the different CPG was also measured.

These permeability measurements allowed, for the first time, to rank the materials of the most commonly used type-5 CPG in North America into distinct clusters corresponding to the different kinds of materials (MP, SMS, SMMS/SMMMS, FS), regardless of the manufacturing company. Separated material groups were also observed from the collection efficiency measurements, but with some differences. In particular, the SMS materials showed very different collection efficiency from each other, i.e., between 45% and 99%. These differences were explained by microscopic analysis and by the physical characterizations of the media. Given that air and vapour permeability are factors correlating with thermal comfort, all these results, constitute a first important step for the choice of the most suited CPG against solid aerosols for a given workplace.

* S = Spunbound, M = Metlblown.

1CM.6

Control of Cooking Oil Fume Emission by the Combination of an Ionic Air Purifier and Bed Filter Packed with Recycled Wastes. Kuo-Pin Yu, Xuan-En Yang, Yen-Chi Chen, CHUN-HSUAN BAI, *National Yang-Ming University*

This study investigated the removal of cooking oil fume by using bed filter packed with 100 gram of recycled waste materials, including tea leaf (TL), wood dusts (WD), rice hulls (RH) and coffee grounds (CG).The removal efficiency of bed filter for particles larger than 1 µm was higher than 95%. For the removal of submicron particles, the ranking of the packing of the performance of the testing materials was in the order of RH, WD, CG, and TL. Ionic air purifier can enhance the removal efficiency of bed filter on submicron particles, particularly the CG filter. The removal efficiency of volatile organic compounds by bed filter ranged from 18.22 to 30.17%.

1CM.7

Combined Effect of Aerosol Concentration and Humidity on Laboratory Filter Loading Experiments. QISHENG OU, David Y. H. Pui, *University of Minnesota*

Current air filter test standards and laboratory evaluations employ artificial testing aerosols to assess filter performance. Solid particle size distribution was found to significantly affect filter lifetime, so it is often reported specifically in reports and literature, together with other operational parameters, such as filtration velocity, temperature, and pressure if applicable. Test aerosol concentration and humidity are another two factors that may affect filter performance, however, in a long time, enough attention has hardly been paid. In order to achieve reasonable test durations, laboratory filter loading tests are often accelerated with aerosol concentration much higher than real application in the field, which is particularly true for filters facing ambient air, such as those in air intake, HVAC, or air cleaning applications. Although suspicious, it is often accepted that the orders of magnitude difference in concentration (μg/m^3 in field vs. mg/m^3 or even g/m^3 in laboratory) has negligible impact on filter lifetime. Relative humidity (RH) was found to affect filter holding capacity, especially for those loaded by hygroscopic aerosols. Unfortunately, humidity is often not controlled, monitored, or reported in literature even when hygroscopic salt particles present.

In this study, the effect of aerosol concentration and test humidity is experimentally evaluated by loading air intake filter media with hygroscopic salts at varied concentrations and RHs. Besides potassium chloride as a typical laboratory salt, ammonium sulfate and ammonium nitrite, which are more abundant in atmosphere, are employed to better represent ambient particle speciation. At same concentration level, filter holding capacity increases with RH increasing as long as particles kept “dry” below their deliquescent RH, which is mainly attributed to the morphological change on particle dendrite and cake due to moisture-salt interaction by capillary condensation. This effect is more pronounced at lower concentration as more time is allowed to develop towards a steady state, which is very difficult to reach from observation in this study. The rate of morphological change competes with the loading rate, so that the observed pressure drop evolution during a loading test represents a combined effect of aerosol concentration and testing RH. At high RHs, where rapid interaction between salt and moisture occurs, the effect of concentration becomes significant. Particles with different hydration-dehydration cycles response differently to RH and concentration level. Detail discussion will be given in the presentation.

1CM.8

Effect of Pore Structures on Filtration Performance of Diesel Particulate Filters Based on 3-D Simulation.

CHENG CHANG, Qisheng Ou, Yun Liang, David Y. H. Pui, *University of Minnesota*

Diesel particulate filters (DPFs) are widely used on diesel engines after-treatment system to mitigate the particulate matter emission. It was found experimentally that pore structures of DPF substrate greatly affected its pressure drop and filtration efficiency. Efforts have been made to correlate substrate pore structure and its filtration performance employing numerical simulations. A large number of numerical methods have been developed to simulate the filtration process, however, mainly based on modeled pore structures which could not sufficiently present the realistic structure of filter substrates. 3-D simulation of DPF performances is rarely reported. In this study, the pore size distribution and porosity of substrates were measured by both mercury porosimetry and X-ray micro-computed tomography (μ-CT). The filtration performance of DPFs was further predicted based on the 3-D micro-structure from μ-CT scans, which was compared with the experimental characterizations. Substrates with different pore structures were then established, from which the effect of porosity and pore size distribution on the particulate deposition in the substrates and filtration performance was further discussed. The results showed that there was a good agreement between the predicted values and experimental results. The most penetrating particle size varied with pore size distribution. In addition, the operational conditions, such as testing temperature and velocity, were found to significantly influence the filtration efficiency.

1DU.1

Optical and Electronic Properties of Flame-Synthesized Carbon Nanoparticles. CHIARA SAGGESE, Ajay V. Singh, Lucy Kaye, Hai Wang, *Stanford University*

Combustion-generated aerosol (soot) or smoke is a notorious air pollutant with hazardous effects on human health and wide-ranging impacts on regional and global climate. Nevertheless, it was only recognized very recently that nascent flame soot particles, i.e., those intercepted during early stages of formation, exhibit fascinating optical and electronic properties, which can be exploited for potential applications in energy conversion and medical diagnostic [1, 2].

In this work, carbon nanoparticles (CNPs) with sizes around 10 nm are synthesized using a series of laminar premixed burner-stabilized stagnation flames [3] and CNPs properties are characterized through UV-visible absorption spectroscopy and fluorescence spectroscopy.

CNPs are collected thermophoretically onto quartz slides at various distances from the burner surface. UV-visible absorption spectra of the particle samples are collected and analyzed in terms of Tauc optical bandgap thus allowing a quantification of the apparent optical bandgap for as-synthesized particles. The results demonstrate the dependency of the optical bandgap on particle size. Fluorescence is observed in the wavelength range of 400-650 nm from particles suspended in organic solvents. Analysis of fluorescence excitation-dependency is carried out and the influence of the solvent is investigated. Implications of these findings will be discussed.

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1DU.2

Graphene Nanosheets Produced via Controlled Detonation. Functionalities with Oxygen/Precursor Ratio. ARJUN NEPAL, Justin Wright, Stefan Bossmann, Christopher Sorensen, *Kansas State University*

Systematic studies of the controlled detonation method for the production of nanoscale graphene to determine the role of oxygen content in pre-detonated oxygen/precursor mixtures are presented. Various ratios of hydrocarbon (acetylene and ethylene) and oxygen are used. The resulting graphene is characterized with BET surface area and porosity, Raman and FTIR spectroscopy, TEM and etc. The specific surface area increases with oxygen content, consistent with Raman measurements that indicate less layering. Spectroscopic measurements of the ca. 10 msec detonation flash indicate black body temperatures are also affected by the oxygen/precursor ratio and overlaying emission lines hint at the mechanisms for the graphene production.

1DU.3

Particle Formation in Combustion Environments: Importance of Charge Distributions on Evolution of Aerosol Size Distributions. YANG WANG, Girish Sharma, Michel Attoui, Pratim Biswas, *Washington University in St Louis*

Combustion systems result in the production of particles both inadvertently and intentionally. The evolution of the size distribution is an important factor in both cases - either for the control of emissions of particles or for the production of novel materials. Charging in flames significantly affects the properties of the particles produced because of its influence in almost all stages of particle formation. In situ measurements with enhanced particle detectors in a premixed flat flame showed that up to 95% of the flame-generated sub-3 nm particles were charged at a sampling height of 5 mm above the burner, indicating the existence of a strong ionization process. The flame-generated ions play an important role during particle inception, as shown by the attachment of ionic species on the particles. Hence, the charging process and the resultant aerosol charge distributions should be considered in aerosol dynamics modeling to accurately predict the behavior of the high-temperature aerosol system. First, this is contrary to reports that most particles below a certain size (~ 5 nm) are not charged. Second, existing models do not consider particle charging, which may lead to a bias in the calculated size distributions.

In this study, Fuchs' charging theory was coupled with aerosol dynamics models to investigate the influence of charging on the evolution of aerosol size distributions in combustion environments. A monodisperse particle growth model and a model using the method of moments were developed and compared in simulating the simultaneous particle charging and coagulation at high temperatures. In order to quantify the charging characteristics of nanoparticles, a high-resolution DMA was used to measure the mobilities of ions generated from a premixed flat flame operated at various conditions. The effect of temperature on ion-particle and particle-particle combination coefficients was further examined. The proposed models showed that the influence of charging on particle growth dynamics was more prominent when the ion concentration was comparable to or higher than the particle concentrations, a condition which may be encountered in flame synthesis and solid fuel-burning. Simulated results also showed that unipolar ion environments strongly suppressed the coagulation of particles. In the end, a simplified analysis of the relative importance of particle charging and coagulation was proposed by comparing the characteristic time scales of these two mechanisms.

1DU.4

Crystal Structure and Surface Composition of Coalescing Ag-Au Nano-Alloys by Molecular Dynamics Simulations.

EIRINI GOUDELI, Sotiris E. Pratsinis, *University of Minnesota*

Bimetallic nanoparticles exhibit catalytic, optical, electronic and magnetic synergy between their constituents. Typically, that synergy is traced to the structure and surface characteristics of such particles. Core-monolayer shell bimetallics exhibit often unique properties that are not an interpolation between those of their parent metals. This behavior is attributed to the lattice mismatch (strain effect) and charge transfer between layers (ligand effect) resulting in different electronic properties. Furthermore, the addition of an ad-metal may alter also the reactant adsorption geometries (ensemble effect) and the degree of ad-metal coverage and its diffusion into the bulk alter the adsorbate binding energies. Yet, there is only limited understanding of the structure and mixing of the two parent metals. Furthermore, understanding metal-adsorbate interactions is a key issue to controlling and improving the functionality of bimetallic nanoparticles in energy applications. Adsorption, however, depends on nanoparticle morphology.

Here, the effect of temperature and initial particle morphology on the sintering rate and crystalline structure is elucidated during sintering of such silver-gold nanoparticles by Molecular Dynamics (MD) simulations. The MD method is validated by the attainment of the melting temperature of pure Ag (Buesser and Pratsinis, 2015), Au (Goudeli and Pratsinis, 2016) and Ag-Au bimetallic nanoparticles as function of their size. The sintering rate of particle pairs with different initial morphology (Ag-Au alloys, segregated or Ag@Au and Au@Ag core-shell nanoparticles) is determined by tracking the evolution of the total surface area and the changes in surface composition of the formed nanoparticle are elucidated during coalescence at T = 500 – 1000 K. The XRD pattern of Ag-Au nanoparticle composites is calculated and compared with experiments (Sotiriou et al., 2014) while their crystallite size is obtained by fitting these MD-obtained XRD patterns (Goudeli and Pratsinis, 2017).

Pure Ag and segregated Ag-Au nanoparticles have larger XRD size than pure Au or alloyed Ag-Au ones. This can provide indication of the detailed structure of flame-made nanoparticles at the atomistic level as experimental measurements of Ag-Au particle size revealed smaller XRD diameter than pure Au or Ag particles (Sotiriou et al., 2014). Furthermore, sintering of Ag@Au core-shell nanoparticles leads to slight reduction (less than 10%) in Ag surface composition, in contrast to Au@Ag ones that increase their Ag surface composition more than 20%.

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1DU.5

Synthesis of $Li_{1.2}Mn_{0.54}Ni_{0.13}Co_{0.13}O_2$ via Low Temperature Flame Spray Pyrolysis. JOSE MADERO, Kuan-Yu Shen, Jeremy Wojtak, Tianxiang Li, Richard Axelbaum, *Washington University in St. Louis*

Lithium, manganese-rich layered cathode material (LMR-NMC) has been studied intensively in the past decades and is one of the most attractive cathode materials under research. Its ability to reach discharge capacity above 200 $mAhg^{-1}$ and low cobalt content make it a promising candidate for cathode material of electric vehicles. Flame spray pyrolysis has been utilized to synthesize LMR-NMC, however, the material is sensitive to the flame conditions as high temperature may lead to additional phase formation. Herein, a low temperature flame spray pyrolysis (FSP) is proposed for the synthesis of $Li_{1.2}Mn_{0.54}Ni_{0.13}Co_{0.13}O_2$. High water content ethanol was used as a fuel and a swirl-stabilized burner was used to achieve the low reactor temperature which is unlikely to be attained via traditional FSP. The effects of reactor temperature, which is controlled via altering ethanol concentration, on the physical properties and the electrochemical performances of the synthesized materials were characterized. The results indicated that as the flame temperature increased, more distinct Li_2MnO_3 phase (C2/m) was grown and larger primary particles were formed. $Li_{1.2}Mn_{0.54}Ni_{0.13}Co_{0.13}O_2$ synthesized with 25 wt % ethanol showed the best results and delivered a discharge capacity of 203 $mAhg^{-1}$ after 100 cycles under C/3. It also achieved good rate capability showing 201 mAhg -1 and 169 mAhg -1 under C/2 and C/1. These results are comparable to the ones demonstrated by $Li_{1.2}Mn_{0.54}Ni_{0.13}Co_{0.13}O_2$ produced via furnace spray pyrolysis and the state-of- the-art co-precipitation.

1DU.6

Effects of Droplet Diameter and Flame Temperature on Nanoparticle Formation Mechanisms in Liquid Aerosol-Fed Non-Premixed Gas Flames. CHRISTOPHER ABRAM, Maksim Mezhericher, Howard A Stone, Yiguang Ju, *Princeton University*

The formation routes of metal oxide nanoparticles are experimentally investigated in self-sustaining gaseous flames fed by aqueous metal-nitrate solution aerosol droplets. To understand the influence of the precursor droplet diameter on the product particle size and morphology, two different atomisation methods are compared: (1) a novel bubble/gas jet atomisation technique, which generates droplets in the sub-micron range with a number mean diameter of ~200 nm; and (2) conventional ultrasonic atomisation producing droplets with a corresponding diameter of ~3.5 µm. Solution droplets consisting of yttrium and europium nitrate salts dissolved in water are delivered to non-premixed CH_4/N_2-O_2 flames to synthesise Eu-doped Y_2O_3 phosphor particles. The product particles are characterised using SEM, TEM, BET gas adsorption and luminescence spectroscopy. Flame temperatures are measured using planar laser Rayleigh scattering.

Depending on the synthesis temperature, the results show that product particles are formed via two different mechanisms: droplet-to-particle and gas-to-particle. At low flame temperatures (1150 K), sub-micron droplets produce cubic-phase luminescent Y_2O_3:Eu^{3+} nanoparticles via the droplet-to-particle mechanism. The particle size can be controlled from 10 to 100 nm by adjusting the precursor concentration in the 0.01-1 mol/L range. Increasing the flame temperature (1450-2750 K) leads to the formation of nanoparticles with a size 3-5 nm via nucleation and growth in the gas phase. In separate experiments, the aerosol flow was also electrically-preheated to 500 K in order to evaporate the solvent upstream before delivery to the flame. With preheating, under the same high temperature flame conditions, the droplet-to particle formation route dominates instead and very few nanoparticles are formed from the gas phase. This result suggests that even for these non-volatile metal nitrate precursors, vaporisation of the precursor occurs predominantly during the extremely rapid droplet drying when the droplets are exposed to the high temperature gradients in the flame. In such cases, specific surface area measurements of the product powders show that sub-micron droplets form an increased fraction of nanoparticles from the gas phase compared with micron-size droplets, because the greater developed surface area of sub-micron droplets enhances vaporisation of the metal precursor.

Analysis of the relevant timescales indicates that the relative rates of solvent evaporation and bulk solute diffusion are dependent on the droplet size. Electron microscopy confirms that dense particles are formed from sub-micron droplets, even when subjected to a rapid rate of gas temperature increase in the flame ($5x10^4$ K/s). For the same synthesis conditions, micron-size droplets tend to form hollow particles because relatively slow solute diffusion causes precipitation on the droplet surface. In this case either slow preheating of the aerosol upstream of the flame or high downstream peak temperatures near the product melting point (>2700 K) are required to promote dense particle formation.

1DU.7

Pursuing Complex Materials Synthesis by Flame Spray Pyrolysis with Advanced Diagnostics. JOSEPH LIBERA, Stephen Cotty, Theodore Krause, Robert Tranter, Jan Ilavsky, Karena Chapman, Gregory Krumdick, *Argonne National Laboratory*

A Flame Spray Pyrolysis reactor has been commissioned at Argonne National Laboratory for research in materials synthesis. The system features a closed combustion environment with full control of all combustion gases and liquids and includes a high-temperature-residence-time section for post-flame in-situ annealing. The system includes in-situ particle and flame diagnostics: PLIF (planar laser induced fluorescence) and SMPS (scanning mobility particle sizing). The PLIF instrument has been configured to provide FRS (filtered rayleigh scattering) temperature and multiple species imaging (Fe, FeO, OH, SiO, NO, Fe, CH, Li). In addition, combustion solid particles are collected before and after the HTRT section for TEM, and advanced synchrotron diagnostics (PDF-SAXS-WAXS). The system has been deployed for the development of Fe-silica catalyst and doped-LLZO for solid state electrolyte applications. We will present preliminary results of the process development demonstrating the use of the in-situ and ex-situ diagnostics for generating useful particles in flame aerosol combustion.

1DU.8

Two-dimensional Diagnostic of Nanoparticle Formation and Transport in Complex Flames Using Phase-selective Laser-induced Breakdown Spectroscopy. YIYANG ZHANG, Yihua Ren, Shuiqing Li, Stephen Tse, *Tsinghua University*

Recently, a diagnostic technique named phase-selective laser-induced breakdown spectroscopy (PS-LIBS) has been developed, especially aiming at tracing nanoparticle formation and transport in reactive flows. PS-LIBS uses the gap between the breakdown thresholds of gas phase and nanoparticles. By creating nano-sized plasmas around particles without ionization of gas molecules, the technique is able to reveal information from particles while the gas phase is not disturbed. In this study we present our recent work on extending PS-LIBS to two-dimensional imaging and related applications for investigating nanoparticle formation and transport in complex flames. Benefited from the non-spark feature, PS-LIBS can be extended to two-dimensional imaging with bandpass filters, which can not be realized in conventional LIBS measurement. We visualize the quick formation of nanoparticles across the flame sheet, as well as particle transport after the flame. Parametric study shows that the intensity of atomic spectra scales linearly with particle volume fraction. Here we will show two particular examples of two-dimensional PS-LIBS imaging. First, a close-up imaging is used to study particle transport near the stagnation plane of a counter-flow flame. The spatial resolution reaches 10 μm. The measured profile of particle concentration remarkably agrees with the numerical solution of particle transport equation. Another example is single-shot two-dimensional imaging in a turbulent co-flow diffusion flame. The snapshots successfully capture particle concentrate near diffusion flame sheet and diffusion/entrainment to the precursor-free side. The single-shot two-dimensional PS-LIBS imaging can be a powerful tool to study turbulent flame synthesis.

1IA.1

Seasonal Variation in the Composition of Submicron Indoor Aerosols of Outdoor Origin. Anita Avery, Michael Waring, PETER DECARLO, *Drexel University*

Outdoor-originated aerosols play a key role in indoor air quality, especially in indoor spaces without strong sources. Since outdoor aerosol varies both spatially and temporally over short (diurnal) and long (seasonal) time scales. We examined the effect of these changes in aerosol loading and chemical composition on indoor aerosol, by examining both indoor and outdoor aerosols in real time in an urban classroom in winter and summer seasons, using an aerosol mass spectrometer (AMS) and a suite of gas phase instruments. Factor analysis of the organic aerosol components identified 3 factors in common between seasons, including hydrocarbon-like, cooking, and oxidized organic aerosol (HOA, COA, and OOA). We report a sulfate-normalized indoor-outdoor ratio (I/O)i/SO4 to account for seasonal differences and variation in ventilation (HVAC operation) to elucidate emissions and chemically-based loss processes between environments. Outdoor aerosols transported indoors in wintertime experience an increased environmental temperature which can drive off water and volatile components, while in summertime aerosols experience a decrease in temperature upon transport indoors and the reverse can happen. However, the degree to which any effect is observed is dependent on the starting (outdoor) aerosol population and the magnitude of change (in temperature, RH, etc.). The median (I/O)i/SO4 values for nitrate, black carbon (BC), total organics, and HOA were smaller in wintertime when temperature gradients between environments favored losses of volatile components; (I/O)i/SO4 values greater than one indicated indoor sources (or less loss) of HOA, BC, and COA. Calculated aerosol liquid water (ALW), as a function of the environmental conditions (temperature and humidity) and the relative contribution of hygroscopic components, varied significantly by season with higher levels in the summertime providing the possibility of aqueous or otherwise liquid processing. This work describes the linkages between chemically-specific variations in exposure between seasons.

1IA.2

Chemically-Resolved Particle Mass Composition in a Swedish Residence Assessed by a Time-Of-Flight Aerosol Mass Spectrometer.

YULIYA OMELEKHINA, Axel C. Eriksson, Patrik Nilsson, Joakim Pagels, Aneta Wierzbicka, *Lund University, Sweden*

A number of deleterious health effects have been identified from exposure to outdoor airborne particulate matter. Given that in developed countries we spend majority of our time indoors, in private homes about 65 % (Brashe et al., 2005), the understanding of this exposure is important, yet knowledge is sparse. Particle levels indoors are affected by indoor sources, infiltration from outdoors or particle mass forms through reactions of gas-phase precursors emitted both indoors and outdoors (Morawska et al., 2013). The aim of this work was to characterize a chemical composition of particle mass indoors, and to gain a better understanding about major contributors to the observed indoor levels with Aerosol Mass Spectrometer. We aimed to identify mass spectral signatures of specific indoor sources. This is preliminary results of measurements for a 1-month period.

Indoor and outdoor measurements were performed in an occupied residence in Malmö, Sweden. It was a naturally ventilated four-room apartment (292 m^3), located in a three-store concrete building surrounded by a green zone. A Time-of-Flight Aerosol Mass Spectrometer (DeCarlo et al., 2006) was used to measure particle mass loadings and size-resolved mass distributions (50-500 nm) of indoor and outdoor chemical species. An automatic switching valve alternated between indoor and outdoor lines with a time interval of 20 and 10 minutes, respectively. Both sampling lines were mounted at the ground floor level and led to the basement where the aerosols were dried and measured by AMS.

Our results showed higher total average mass concentration indoors (12.9 µg/m^3) compared to outdoors (5.4 µg/m^3) over the entire measuring period. Indoor to outdoor (I/O) ratio for organics was 6.7, for sulphate 0.5, for nitrate 0.3, for ammonium 0.2 and for chloride 0.2. The dominant species indoors was organic matter, accounting for most of the total particle mass (92 %) due to contribution from indoor sources and from outdoor infiltration. Non-volatile sulphate showed reduced infiltration from outdoors. From comparison of outdoor and indoor concentrations of ammonium nitrate and ammonium chloride, which are sensitive to temperature and RH (Lunden et al., 2004), a clear reduction due to phase change was observed upon outdoor-to-indoor transport. We investigated different organic mass spectra for indoor events as recorded in the logbooks. The main events analysed comprised from various types of cooking and candle burning. They showed to emit different proportions of hydrocarbons and oxygenated organic species, which yield $C_xH_y^+$, $C_xH_yO^+$, $C_xH_yO_z^+$ ion classes. The relative intensity of $C_xH_y^+$ ion class out of the total organic signal during frying was 65-68 %, deep-frying ~ 68 %, baking 60-70 %, other forms of cooking 60-68 %, candle burning 60-70 %. For $C_xH_yO^+$ ion class: frying 25-30 %, deep-frying 24-25 %, baking 27-32 %, cooking 25-31 %, candle burning 20-30 %. For $C_xH_yO_z^+$ ion family: frying 7-8 %, deep-frying 7-8 %, cooking and baking 6-9 %, candle burning 6-8 %.

The observed variability in organic mass spectral signature for different indoor sources should allow us to apply Positive Matrix Factorization for source apportionment and processes occurring in indoor air. This will help us to gain a better understanding about main contributors to the observed loading indoors.

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1IA.3

Evaluation of the Molecular Composition of Particle- and Gas-Phase Material in an Indoor Residential Environment using Positive Matrix Factorization. CLAIRE FORTENBERRY, Michael Walker, Audrey Dang, Arun Loka, Gauri Date, Karolina Cysneiros de Carvalho, Glenn Morrison, Brent Williams, *Washington University in St. Louis*

Natural ventilation (e.g., window opening and closing to regulate indoor temperature) promotes infiltration of outdoor pollutants and oxidants into the indoor environment, and infiltrating oxidants like ozone (O_3) can drive formation of new pollutants through oxidative chemistry [1]. Changes in air exchange rates with window opening can also drive volatilization and resuspension of deposited material. Many common indoor air pollutants are semi- or intermediately volatile and therefore actively partition between the gas and particle phases. Because respiratory deposition depends on chemical and physical properties like diffusivity and particle mobility diameter [2,3], greater understanding of pollutant phase partitioning is needed to improve exposure estimates and inform residential building standards.

The Air Composition and Reactivity from Outdoor aNd Indoor Mixing (ACRONIM) field campaign was conducted in the summer of 2016 at a single-family residence in St. Louis, Missouri. A Thermal desorption Aerosol Gas chromatograph (TAG), which pairs automated aerosol collection with thermal desorption and online analysis by gas chromatography-mass spectrometry (GC-MS) [4], was used for chemical measurements of indoor particles and gases. Samples were collected alternately indoors and outdoors with two-hour time resolution throughout the study under three major natural ventilation conditions (all windows closed, one window open, two windows open). A denuder difference method, wherein the TAG sampled alternately through a diffusion denuder and a bypass line, was used to determine the relative contributions of gases and particles to compound abundances.

Using mass spectral databases, we identified approximately 200 compounds in indoor and outdoor ambient TAG samples. A subset of these compounds spanning a range of volatilities and chemical functionalities were integrated, and positive matrix factorization (PMF) analysis was used to identify co-varying compounds across the measurement period. A three-factor PMF solution resolved one indoor factor, one outdoor factor, and one factor corresponding to indoor compounds enhanced with window opening. Compounds loading into the enhanced factor include indoor-originating phthalates and esters common in personal care products, indicating increased volatilization of deposited material with changes in air exchange rate. Loading of acids and aldehydes into the enhanced factor indicate formation of compounds through oxidative chemistry. Higher-factor PMF solutions provide improved resolution of outdoor-originating compounds, including polycyclic aromatic hydrocarbons (PAHs) associated with combustion. Finally, by assessing differences between denuded and undenuded compound abundances, we found that many compounds measured by the TAG in the indoor environment exist significantly in the gas phase, with less than 40% of the inte-grated compounds exhibiting a particle-phase fraction greater than 0.5.

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1IA.4

Study of Particulate and Gas-phase Pollutants Emitted from Household and Personal Care Products Under Various Heating and Combustion Scenarios. DONNA AUGUSTE, Shelly Miller, *University of Colorado at Boulder*

In this quantitative research study we investigated fine particle, VOC and PAH emissions from household and personal care products. The products were selected for investigation after Denver-area African American families with asthmatic children identified the products as potential asthma triggers in their homes by using low-cost real-time indoor air quality sensors. We tested the products by using thermal desorption techniques in a controlled lab setting. Because some of the products were selected on the basis of gas-phase pollutants that were emitted when the products were heated or burned, such as hair styling products heated by a flat iron or burned with a butane lighter, we tested the products and documented emissions in a wide range of heating and combustion scenarios. Outcomes of this study may provide data for researchers who are evaluating the impact of household and personal care products on residential indoor air quality for people who are vulnerable due to health conditions.

1IA.5

Characterization of Aerosols in the International Space Station. MARIT MEYER, *NASA Glenn Research Center*

Maintaining good air quality in the International Space Station (ISS) presents unique challenges. Until recently, the environmental monitoring within the ISS has prioritized gaseous constituents. Elevated CO_2 levels and other contaminants were deemed a more immediate health threat to the astronauts who are of excellent health. Although particulate matter (PM) requirements exist, aerosols in the ISS cabin have not been characterized with real-time instruments. NASA's Life Support Systems Project has a roadmap for accomplishing this end goal, which includes intermediate research projects on ISS aerosols. The Aerosol Sampling Experiment was successfully completed in 2017, including sample analysis by microscopy. The re-flight of this experiment in 2018 will provide additional results to compare with the first samples. Additional samples of airborne particulate matter will be obtained in much larger quantities from vacuum cleaner bags. In the absence of gravitational settling, particles are driven by the cabin air flow and deposit on vents and filters of the air handling system. These vents are vacuumed weekly by the astronauts as part of their housekeeping activities. The experiment called Divert Unwanted Space Trash (DUST) will collect debris samples from vents, and vacuum bags will be returned to Earth where various analyses will be performed. This activity also provides the first estimate of PM concentration for ISS cabin air. Plans for a flight experiment with a real-time aerosol instrument are underway, targeting a 2019 launch. Progress of these programs are summarized, along with the latest results from ISS aerosol characterization work.

1IA.6

Indoor Fine and Ultrafine Aerosol Particles Exposure and Its Relationship to the Outdoor Concentrations in Private Homes. Jiangyue Zhao, Birgit Wehner, Thomas Tuch, Kay Weinhold, Maik Merkel, Ulrich Franck, Wolfram Birmili, Anja Lüdecke, Tareq Hussein, Lina Wang, ALFRED WIEDENSOHLER, *TROPOS*

Nowadays people spend a large fraction of their lifetime indoor. Currently, only limited information is available about the exposure of residents to indoor fine and ultrafine particles, which can originate from either indoor or outdoor sources. It is thus important to study the contribution of outdoor sources and residential activities to the indoor air. The efficiency of penetration processes of aerosol particles from outdoor to indoor depends on the particle number size distribution (PNSD), meteorological conditions (e.g. wind speed, temperature), and residential building structure. Therefore, on behalf of the German Environment Agency (UBA), a project to study the indoor aerosol particle exposure and its relationship to the urban and rural atmosphere was granted to the Leibniz Institute for Tropospheric Research (TROPOS).

Measurements are performed in 40 households in two cites of Germany, households are located in the urban, suburban, and rural areas. Each household was or will be probed twice for one week, covering both, the cold and warm seasons. The first measurement period took place in Leipzig in 2017. Measured parameters for indoor and outdoor air have been the PNSD (0.01 – 0.8 µm), using mobility particle size spectrometers (MPSS, designed and build by TROPOS), and PM1, PM2.5, PM10 mass concentrations , using optical particle size spectrometers (Grimm Model 1.108). Additional indoor measurements were the equivalent black carbon mass concentration (microAeth Model AE51), and the indoor CO2 concentration (CO2 sensor, GMP252 Vaisala) to document the room ventilation. The measurements are accompanied by a questionnaire that documents the room characteristics and a digital notebook, capturing the residential activities. During the measurement, a new concept has been designed to determine indoor and outdoor PNSD of fine and ultrafine particles with high quality, as well as measurement of course mode particle mass concentrations. It is designed to perform measurement in multiple private homes over a period of more than one year, to obtain statistically more robust data.

This work presents results from the one-year measurement period in Leipzig, including the variation of particle number concentration (PNC) and I/O ratios in fine and ultrafine particle size ranges, caused by residential activities, as well as the evolution of different indoor particle sources. According to the variation of median of the indoor and outdoor PNCs, the outdoor PNC is generally higher than the indoor one. During nighttime (00:00 - 07:00), both indoor and outdoor PNCs decreased constantly due to less traffic and no indoor emissions. On the other hand, the indoor PNC and I/O ratio show peaks during breakfast, lunch and dinnertime. Ultrafine aerosol particles are especially produced due to cooking activities or candles burning. The 24-h median I/O is in the range of 0.4 to 1, its variation indicate that the indoor aerosol is increasingly decoupled from outdoor during nighttime and during daytime the influence of the outdoor aerosol is more significant (I/O ration close to 1). Black carbon concentrations will be compared to PNC of different size ranges to obtain a better understanding of the black carbon size range from different indoor sources.

1IA.7

Heterogeneous Ozonolysis of Squalene Particles: Gas Phase Products Depend on Water Vapor Concentration. CALEB ARATA, Nadja Heine, Pawel Misztal, Kevin Wilson, Allen H. Goldstein, *University of California, Berkeley*

The oxidation of skin lipids plays an important role in the composition of indoor air. Squalene, $C_{30}H_{50}$, constitutes 10% of the mass of human skin lipids, and contributes 50% of the unsaturated carbon bonds in skin lipids. When exposed to ozone, squalene is quickly oxidized to products spanning a wide range of volatility with some products remaining in the condensed phase while many fragmentation products are released to the gas phase.

Previous work examining the condensed phase products of pure squalene particle ozonolysis in a flow tube reactor found that the rate of squalene ozonolysis was independent of water vapor concentration. However, an increase in water vapor concentration led to lower concentrations of secondary ozonides, increased concentrations of carbonyls, and reduction of particle diameter suggesting water changes the fate of the Crieege intermediate.[1]

To determine if this loss of volume corresponds to an increase in gas phase products, we measured gas phase volatile organic compound (VOC) concentration via proton transfer reaction time-of-flight mass spectrometry (PTR-TOF-MS), a soft chemical ionization technique that allows for quantification of the full suite of oxygenated VOCs which might be expected from these reactions. Our studies were conducted in a flow tube reactor at atmospherically relevant ozone exposure levels (10-30 ppb hr) with pure squalene particles. Along with VOC measurements, the condensed phase composition was measured with vacuum ultraviolet photoionization aerosol mass spectrometry (VUV-AMS) and particle size and number were detected by scanning mobility particle sizer (SMPS).

PTR-TOF-MS measurements indicate that an increase in water vapor concentration leads to a strong enhancement of gas phase oxidation products at all levels of ozone exposure. At high ozone exposure (30 ppb hr), all early generation gas phase products with an unsaturated carbon bond are consumed and known terminal products (acetone, 4-oxopentanal (4-OPA), and succinaldehyde) dominate the gas phase VOC composition across all levels of water vapor concentration. An increase in water vapor from ~3% RH to 70% RH at this high ozone exposure effectively doubles the mass concentration of gas phase products. Even under modest ozone exposure (10 ppb hr), changing water vapor concentration enhances VOC mass concentration by ~70%. At all levels of ozone exposure and water vapor concentration the commonly identified squalene oxidation products (terminal products + 6-methyl-5-hepten-2-one (6-MHO)) account for greater than 75% of the observed mass in the gas phase, and we also detect smaller yields of a complex array of products presumably accounting for the remainder of the mass.

The ability of water concentration to dictate the fate of the Criegee intermediate, and therefore the volatility of the oxidation products, suggests that indoor humidity will affect the concentration of gas phase VOCs emitted from ozonolysis of skin oil. This work also strongly suggests that future heterogeneous alkene ozonolysis experiments should consider the effects of humidity on the products of the reactions.

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1IA.8

Emission and Particle Size Distribution of Polycyclic Aromatic Hydrocarbons in Oil Fumes from Domestic Cooking. YU-CHENG CHEN, Kai-Wei Ke, Chin-Yu Hsu, *National Health Research Institutes, Taiwan*

Cooking oil fume is one of the most important components of indoor air pollutants. This study was to investigate the characteristics and emissions of polycyclic aromatic hydrocarbons (PAHs) in cooking oil fumes generated by stir-frying fish. Gas- and particle-phase PAHs with 22 congeners were analyzed by GC/MS-MS. Particle size distribution of PAHs were also evaluated using Micro-Orifice Uniform Deposit Impactors (MOUDI). The mean concentration of total PAHs was 338±16.0 ng/m^3, where gas- and particle-phase PAHs accounted for 93.6% and 6.4%, respectively. 2- to 4-ring PAHs were predominant. PA, FL, and Pyr were the dominant compounds of PAHs in the cooking exhaust. Particle size distribution (MMAD= 1.01 µm, GSD=4.2) showed that PAHs were mainly concentrated in the fine mode with a diameter <2.5 µm, accounting for 67.4%. The emission factors for total PAHs and BaPeq were 11850 and 29.3 ng/kg-fish.

1IN.1: INVITED

Ice Nuclei and Their Impact on Clouds in Alaska. GIJS DE BOER, Matthew Norgren, Jessie Creamean, Amy Solomon, Maximilian Maahn, Fan Mei, Hagen Telg, Allison McComiskey, *CIRES/NOAA*

Northern Alaska is signifcantly influenced by the presence of ice nucleating particles (INP). These particles have a strong impact on hydrometeor properties in the region, introducing influence on cloud radiative properties, precipitation intensity, and cloud lifetime. While critical to the accurate projection of future climate states, the roles of these particles remain a challenge to understand and quantify. The Arctic is particularly sensitive to these interactions because small changes to the impacts of clouds on surface energy exchange can have large implications on a region known for extensive cloud cover whose atmospheric state exhibits large sensitivities to the surface energy budget, and where small shifts in temperature may result in dramatic departures in the surface energy budget through modification of surface albedos. To better understand the role that INP particles play in this puzzle and the sources of aerosols involved, we are using a variety of observational and modeling tools to gain new insight into the importance of these particles.

In this work, we will present observational analyses that shed light on the interplay between aerosols and cloud microphysical and radiative properties in Northern Alaska. Using measurements from surface-based US Department of Energy (DOE) Atmospheric Radiation Measurement (ARM) program observatories at Oliktok Point and Utquiagvik (formerly Barrow) Alaska, together with airborne measurements, we will cover:

[1] Observations of INP in northern Alaska and the potential sources of these particles,
[2] An observational study demonstrating that aerosol loading plays a role in the modulation of precipitation from mixed-phase clouds, thereby impacting surface albedo and cloud dynamics, and
[3] Modeling work demonstrating that small changes to the balance of INP and Cloud Condensation Nuclei (CCN) can impact mixed-phase cloud structure and lifetime.

This combination of studies will highlight the need to further our understanding of INP in this part of the world.

1IN.2: INVITED

Traces of Ice Nucleation Modes in Arctic Mixed-phase Clouds Simulated by a Habit Prediction Scheme. TEMPEI HASHINO, Gijs de Boer, Hajime Okamoto, Greg Tripoli, *Kyushu University*

Ubiquitous and long-lasting Arctic low-level clouds are known to affect the surface energy budget through radiation especially when liquid particles are present (Curry and Ebert 1990, Hashino et al. 2016, Shupe et al. 2011). However, simulation of the mixed-phase status have been challenging partly due to their large sensitivity on ice number concentration (e.g., Morrison et al. 2011, Young et al. 2017). The ice nucleation modes active in the clouds are still open to question (e.g., Fridlind et al. 2007, Paukert and Hoose 2014). In this presentation, we make contrasts of results obtained with three ice nucleation schemes through 3D LES experiments.

A habit-prediction scheme called SHIPS (Hashino and Tripoli 2007, 2008, 2011ab) was implemented in a scalable non-hydrostatic model, UW-NMS (Tripoli and Smith 2014ab). Three ice nucleation schemes are considered: Meyers deposition-condensation freezing, Bigg-type time-dependent immersion freezing parameterization (Bigg), classical nucleation theory based scheme (CNT). For May 7th case during SHEBA campaign, it was found that large cloud droplets in downdraft freeze actively with Bigg. On the other hand, CNT immersion scheme produces much of ice over updraft where supersaturation is relatively high. This means that the initial size of frozen particles is different among the immersion schemes. Through non-linear feedback built in the habit prediction scheme, the resulting aspect ratios of plates clearly differ each other. As a result, radar reflectivity simulated with Bigg scheme better match with ground radar observation although the ice water paths of the two are similar. In the presentation, we will discuss implication of the volume dependence of freezing and formation of the large cloud droplets.

1IN.3

Variations in Ice Nucleating Particle Concentrations at Four Arctic Locations. HEIKE WEX, Lin Huang, Hayley Hung, Rita Traversi, Rebecca J. Sheesley, Claire Elizabeth Moffett, Tate Edward Barrett, Rossana Bossi, Markus Hartmann, Xianda Gong, Frank Stratmann, *Leibniz Institute for Tropospheric Research, Germany*

Filter samples collected on quartz fiber filters at four Arctic measurement stations, Alert, Barrow, Ny-Ålesund and Villum were analyzed with respect to number concentrations of ice nucleating particles (NINP). Measurements were done following the method proposed by Conen et al. (2012), examining immersion freezing: a filter punch (1 mm in diameter) was put into every one of the 96 tubes of a PCR tray, where each tube contained 50 microliter of pure water; the tray was sealed and immersed in the cooling bath of a thermostat and cooled down with a cooling rate of 1K/min; during the cooling, every 6 s a picture of the tray was taken from above, and discrimination between liquid and frozen droplets was done. The obtained temperature dependent freezing curves were used to derive NINP in the temperature range from -5°C down to -20°C.

For Ny Alesund, samples from spring and summer months were examined, while a yearly coverage existed for the other stations. Differing values of NINP were observed during the year, and in general during summer and fall, particles were more ice active than during winter and early spring, indicating that different sources of ice nucleating particles contributed to the panarctic area, their influence varying with season. The lowest values determined for the Arctic samples were about 1 order of magnitude lower than NINP determined from precipitation samples collected in North America and Europe (Petters & Wright 2015), but the highest values were comparable, pointing at a biogenic origin from either the biosphere (e.g., from fungal spores or bacteria) or from marine sea spray (e.g., from algae or bacteria). These biogenic ice nucleating particles might become more abundant as the Arctic warms, with potential influences on cloud properties as e.g., the lifetime of the persistent Arctic stratiform clouds.

This study gives first insights into yearly cycles of ice nucleating particles in the Arctic, but it also reveals open questions and suggests future pathways concerning their examination.

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1IN.4

The Concentrations, Spatial Distribution, and Compositions of Ice Nucleating Particles in and around Stratiform Clouds over the Southern Ocean. PAUL DEMOTT, Christina McCluskey, Kathryn Moore, Thomas Hill, Ezra Levin, Cynthia Twohy, Lynn Russell, Darin Toohey, Bryan Rainwater, Greg McFarquhar, Alain Protat, Ruhi Humphries, Gerald Mace, Melita Keywood, Roger Marchand, Cory Wolff, Jeffrey Stith, Sonia Kreidenweis, *Colorado State University*

The Southern Ocean is one of the stormiest places on Earth, and is blanketed in frequent clouds whose properties, phase and lifetime are not well represented in climate models, leading to a high bias in predicted radiation reaching the ocean surface (compared to satellite measurements) over a broad latitude range south of about 55° S latitude. These model biases in turn lead to potentially incorrect predictions of ocean and atmospheric feedbacks. The Southern Ocean Clouds, Radiation, Aerosol Transport Experimental Study (SOCRATES), conducted in January and February 2018 in the region between Hobart, Tasmania and 62° S, provided the most comprehensive assessment of aerosol interactions with supercooled and mixed-phase clouds ever compiled over the Southern Ocean. Studies were specially designed to document primary ice nucleation and its influence on cloud phase. These studies provide constraints for follow on numerical modeling studies to explore primary and secondary (ice “multiplication”) ice formation processes in these clouds.

The NSF/NCAR G-V payload for SOCRATES included two types of ice nucleating particle (INP) measurements, a continuous flow diffusion chamber (CFDC) for real-time INP measurements and bulk volume filter collections for offline immersion freezing temperature spectra measurements. Flight plans were designed to quantify the INP budget around clouds and its potential influence on ice formation in clouds. Typically, measurements were first made of aerosols in ambient air just above supercooled cloud layers (sometimes multiple layers were sampled), and then a level leg was flown within the peak cloud liquid water layer to observe cloud microphysics. Cloud residual particles were sampled with a counterflow virtual impactor (CVI) inlet and the residuals collected for further analysis. Finally, a level leg was flown below clouds in the marine boundary layer (MBL) to sample aerosols coming primarily from sea spray emissions. Both ambient aerosols and cloud residual particles were analyzed to determine INP number concentrations. Aerosol collections for compositional analyses were made from each region around clouds, and from activated INPs from the CFDC. Offline treatments on bulk aerosol samples are also planned to investigate contributions from heat labile INPs and organic INPs. These aircraft data were supported by the same INP measurement suite operated on the Australian Marine National Facility ship, the RV Investigator, leading to comprehensive spatial data on INPs in the Southern Ocean MBL.

INP concentrations over the Southern Ocean region were found to be some of the lowest on Earth, both in the free troposphere and in the MBL. CFDC INP measurements focused at water supersaturated conditions were often at detection limits, well below 1 per liter at -30°C. The particle number concentration enhancement (20-40 times) of the CVI inlet thus permitted best INP detection, as did use of an aerosol particle concentrator on the RV Investigator. INP concentration and compositional data will be summarized, relationships to aerosol properties including bioaerosols will be discussed, and a first comparative inspection of INP versus cloud ice particle concentrations and evolution will be presented.

1IN.5: INVITED

Laboratory Studies on Mechanisms Behind Bacterial Ice-Nucleation Activity. Meilee Ling, Heike Wex, Sarah Grawe, Jonas Jakobsson, Susan Hartmann, Jakob Löndahl, Kai Finster, Thomas Boesen, TINA SANTL-TEMKIV, *Aarhus University, Denmark*

Ice nucleation active (INA) bacteria are one type of atmospheric ice nuclei that have attracted particular attention due to their unique ability to produce specific INA proteins (INprot). Several studies have shown that these proteins are the most efficient ice nuclei known as they induce nucleation at temperatures close to 0°C. We have just started understanding the impacts of aerosolized INA bacteria on atmospheric processes. We present the outcome of a study that focused on elucidating the largely unknown molecular mechanisms behind ice-nucleation induced by INA bacteria.

It is known, that ice nucleation in bacteria is induced by certain proteins. These proteins consist of three parts: N-terminal, C-terminal and the central repeat domain. The central repeat domain is involved in ice-formation and is essential for the protein to function as ice nucleating particle. To understand the role of the central repeat domain of the INprot as well as the role of intermolecular interactions between INprot molecules for their ice-nucleation behaviour, we produced purified recombinant proteins with reducted theoretical ice-binding surface. The native protein that contains 67 amino acid tandem repeats was truncated to only contain 9, 16, and 28 amino acid repeats. The recombinant proteins interacted with bacterial lipids to form particles that are between 30 nm and 100 nm in size. The particle size corresponded roughly with the size of the central repeat domain of INprot.

For one of the INprot constructs that contained 16 repeats (INprot16R), ice nucleation assays were performed using both the Leipzig Aerosol Cloud Interaction Simulator (LACIS) and droplet freezing assays. We found that the truncated bacterial ice nucleation protein was ice active although its ice-binding site was more than 4 times smaller than the sizes of native protein. The onset ice nucleation temperature was between −24°C and −26°C, which strongly indicated that the number of amino-acid tandem repeats determined the ice-nucleation temperature. In addition, we demonstrated that ice nucleation between -9°C to -10°C, which was comparable to the ice-nucleation activity of full-length INprot, was caused by large INprot16R oligomers. These results support previous observations that oligomerization of INprot increases their ice-binding surface, thus changing their freezing behaviour. In conclusion, both the repeat number and the degree of oligomerization contribute in an independent manner to the nucleation mechanism of INA proteins.

1IN.6

Field Collected and Synthesized Proteinaceous Material as Ice Nucleating Particles in Immersion Freezing. NADINE BORDUAS-DEDEKIND, Robert O. David, Kristopher McNeill, Zamin Abdulali Kanji, *ETH Zürich*

Organic aerosols represent a subset of atmospheric particles able to act as cloud condensation nuclei (CCN) and, as more recently found, ice nucleating particles (INPs). CCN and INPs affect the ratio of water and ice in mixed-phase clouds, leading to an impact on Earth's radiative balance. In this work, we use dissolved organic matter (DOM) as a proxy for organic aerosols and lake spray aerosols in ice nucleation experiments. DOM is a complex mixture of terpene-derived compounds, proteinaceous material, lignin, organic acids and some ions. As the dominant IN mechanism in mixed-phase clouds is immersion freezing, we investigated the ability of DOM to act as INPs, using our homebuilt DRop freezing Ice Nucleation Counter Zurich (DRINCZ). We use field collected DOM from American rivers and find that the DOM, despite coming from different locations, shows consistent freezing around –12 °C. We are currently extending these results to field collected snow samples in Switzerland. In addition, we identify the material within DOM responsible for its INP activity. Preliminary results suggest the importance of proteinaceous material and so current work includes synthesis of discrete proteins of different sizes to probe their ice nucleating potential. A laboratory-based chemical perspective to the ability of proteinaceous material to nucleate ice will be presented.

1IN.7

The Importance of Biogenic Material to the Ice Nucleating Particle Concentration in a Coastal Tropical Site. LUIS ANTONIO LADINO, Graciela Raga, Harry Alvarez-Ospina, Manuel Andino, Irma Rosas, Leticia Martinez, Eva Salinas, Javier Miranda, Zyanya Ramirez, Bernardo Figueroa, Erika Quintana, Luis Maldonado, Agustin Garcia, Cédric Chou, Victoria Irish, Allan Bertram, *Universidad Nacional Autónoma de México, Mexico City, Mexico*

Recent studies have demonstrated that oceans can emit aerosol particles with the capability to nucleate ice in clouds known as ice nucleating particles, INPs (e.g., Wilson and Ladino et al., 2015; DeMott et al., 2016; Ladino et al., 2016; and McCluskey, et al., 2017). This is very relevant information that can be included in climate and weather models to predict the formation of ice in clouds given that most of them do not consider the oceans as a source of INPs. There is a need to conduct field measurements in tropical latitudes, since most of the past and recent studies have been conducted in mid- and high latitudes, to understand the role that marine aerosol play in the hydrological cycle and climate of tropical regions.

The present study shows the results obtained in a field campaign conducted in the village of Sisal, located on the coast of the Yucatan peninsula in Mexico (21°09’55”N 90°01’50”O) in January 2017, the first measurements obtained at this tropical site and one of the few data sets at similar latitudes. Aerosol particles around Sisal were found to be very efficient INPs, with onset freezing temperatures as high as -3°C (in some cases), similar to the onsets of Pseudomonas Syringae (Wex et al. 2015) or Arctic sea surface microlayer waters (Wilson et al., 2015).

The results show that the INPs concentration in Sisal is higher than in other studied locations using the same INP counter type. Surprisingly, the air masses arriving in Sisal after the passage of cold fronts reported higher INP concentrations than the average value for the whole sampling period, despite the low total aerosol concentration.

Given the large concentration of INPs at -15°C, it can be inferred that biological particles are very important in ice cloud formation in this tropical location. A variety of microorganism were identified by Gram staining analysis and by detailed bacterial strain isolation. Although the majority are of terrestrial origin, some of them are clearly oceanic, indicating that marine aerosol particles could also play a big role in cloud formation, especially in the presence of cold fronts.

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1IN.8

Biogenic Macromolecules from Terrestrial and Marine Biospheres Acting as Ice Nucleating Particles. DANIEL KNOPF, Joseph Charnawskas, Peter Aaron Alpert, Josephine Aller, Swarup China, Daniel Veghte, Daniel Bonanno, Alexander Laskin, Ryan Moffet, Mary Gilles, Jian Wang, *Stony Brook University*

The terrestrial and marine biospheres are sources of ice nucleating particles (INPs) active in the immersion freezing and deposition ice nucleation modes. In regions where mineral dust is scarce, biogenic INPs may control cold cloud formation. Atmospheric particles collected i) in the marine environment including surf zones and Pacific and Atlantic oceans in addition to laboratory mesocosm experiments with natural seawater, ii) above and below the forest canopy in the Amazonian region during the Green Ocean Amazon campaign, and iii) at the ground site of Graciosa Island during the Aerosol and Cloud Experiments in Eastern North Atlantic campaign are examined for their ice nucleation ability. Particles were collected on various substrates for micro-spectroscopic single particle chemical analyses using size-resolved impaction. Ice nucleation experiments were conducted covering temperature and humidity conditions for mixed-phase and cirrus clouds. Experiments were accompanied by scanning electron microscopy with energy dispersive X-ray spectroscopy SEM/EDX for elemental and morphology analyses of particles including INPs, and scanning transmission X-ray microscopy with near edge X-ray absorption spectroscopy (STXM/NEXAFS) for particle mixing state analysis. Additionally, sea spray aerosol (SSA) particles were photospectroscopically examined for the presence of polysaccharidic and proteinaceous matter following chemical analyses.

Analyses of ambient particles including INPs by STXM/NEXAFS show that the organic matter, often present as a coating, is very similar among biogenic particles from different sources. The widespread presence of polymeric carbohydrate molecules is corroborated, in the case of SSA particles, by staining and photospectroscopic analyses. Corresponding ice nucleation experiments with collected particles find that deposition ice nucleation and immersion freezing are initiated under very similar conditions of temperature and humidity. The observations of similar chemical composition and ice nucleation propensity for particles from both the marine and terrestrial biospheres suggest that naturally occurring biogenic polysaccharidic macromolecules from photosynthetic-active plants and phytoplankton form amorphous polymers that may play a role in cloud glaciation under atmospheric conditions. These findings support previous studies showing that ice nucleating macromolecules (INMs), which can be polysaccharides, demonstrate freezing temperatures that correlate with the size of the INMs according to classical nucleation theory.

1MD.1

Verifying the Hygroscopic Particle Growth Model during the Time Relevant to Lung Inspiration. PATRICK O'SHAUGHNESSY, Ralph Altmaier, Ross Walenga, Ching-Long Lin, *University of Iowa*

Under high humidity, hygroscopic compounds attract, absorb, and retain water molecules resulting first in deliquescence, during which the salt core dissolves and a film of salt solution increases, followed by an increase in the resulting droplet solution up to an equilibrium size. The human airways provide an environment suitable for hygroscopic particle growth which will ultimately affect their deposition sites. This research is therefore motivated by the need to accurately determine deposition sites of pharmaceutical compounds that alleviate airway diseases with the use of computational fluid dynamic modeling of the human lung. A set of published coupled differential equations for predicting droplet growth and droplet temperature change were used to predict the growth of sodium chloride particles. Sodium chloride was used as the test substance because its properties to be incorporated into the growth model are well known and accurate. The added effect of salt core dissolution during the initial fast growth phase of the particles was also explored. Differential equations were solved using the MATLAB ordinary differential equation solver function (ODE45). Experimental validation of the model was accomplished with the novel use of video photography to measure frame-by-frame the growth of a salt particle on a microscope slide placed on an inverted light microscope. Using an apparatus containing computer-activated solenoid valves, room air was instantly replaced with air of a known humidity and the subsequent growth of the particle was then videotaped. The numerical model was validated through comparison with the experimental data over the initial 0.2 seconds of growth, consistent with the average residence time needed for transport of air from the top of the trachea to the first lung bifurcation. The experimental data indicated an initial growth phase that is consistent with the model when adjusted to simulate the dissolution of the salt core. This was achieved in the model by holding the solution concentration of the film of salt solution surrounding the salt core at saturation until the droplet grew to have a volume sufficient to hold the entire mass of the original salt particle in solution at saturation. The conventional hygroscopic model then proved to be sufficiently accurate when modeling further growth of the homogeneous salt solution droplet to its equilibrium size. Without incorporating model enhancement to account for salt core growth, the hygroscopic growth model overestimated droplet diameter by an average of 32.1% compared to the measured values during the time span < 0.2 sec. When incorporating salt core growth, the modeled values slightly underestimated droplet diameter by -3.1% over that time span. The deliquescence phenomenon during which the salt core dissolves is therefore a critical component missing from currently published particle growth models. Future research will incorporate this added aspect of the hygroscopic growth model applied to more complex pharmaceutical compounds.

1MD.2

Regional Lung Deposition of Nebulized Hypertonic Saline for Trans-Nasal vs. Oral Inhalation in Healthy, Non-Smoking Adults. WILLIAM BENNETT, Kirby Zeman, Landon Holbrook, Katie Howe, Jihong Wu, David Busick, Richard Boucher, Scott Donaldson, *University of North Carolina at Chapel Hill*

Background: Nebulized, hypertonic saline (7%) (HS) has been shown to improve hydration of cystic fibrosis (CF) airway surfaces, improving both mucociliary clearance and lung function in these patients. We previously demonstrated by gamma scintigraphy that a transnasal Pulmonary Aerosol Delivery device (tPAD; Parion Sciences, Inc., Durham, NC) is able to deliver a HS aerosol to the lungs as efficiently as a standard oral nebulizer (Pari LC Star) but with slightly more peripheral airway deposition as determined by the central/peripheral (C/P) ratio of deposited activity (Zeman et al, J Aerosol Med Pulm Drug Deliv. 30:223, 2017). Because there is uncertainty in the ability for C/P to accurately characterize airway vs. alveolar deposition we speculated that adding insoluble, particle clearance measures post-initial deposition would improve the resolution of aerosol deposition in the various airway generations of the lung.

Methods: Regional deposition for both devices was characterized by measuring the % clearance of inhaled radiolabelled (Tc99m) sulfur colloid particles (in 7% HS) using gamma scintigraphy over 24 h in healthy volunteers (n=5). The traditional C/P ratio was also calculated from the initial deposition image (normalized to a Cobalt57 transmission image for each subject). Airway deposition within bronchial airways (large, intermediate, and small) was estimated as % clearance of the insoluble labeled particles through 24 hours post deposition (Aw). Within the bronchial airways we estimated regional deposition in large airways as % clearance through 3-hour post deposition (LargeAw); large and intermediate airway as % clearance through 6 hours (Large/InterAw); and small airways as the % clearance between 6 and 24 hours (SmallAw). For both inhalation modalities, spontaneous flows/volumes were measured by a pneumotachograph during exhalation. Particle size for the tPAD was designed to be sufficiently small to minimize nasal deposition [volume median diameter (VMD)=1.3 um], and was 3.1 um for the LC Star.

Results: Mean tidal flows and volumes were similar for breathing on the tPAD vs. LC Star, 0.32 vs. 0.24 L/sec and 0.93 vs. 0.80 L. Both devices achieved similar % lung deposition relative to delivered dose, % lung = 30.7 vs. 35.4 for the tPAD vs. LC Star. Percent (%) extrathoracic deposition was also similar = 8.1 (tPAD) vs. 5.7 (LC Star). While the C/P ratios for the initial deposition were not different, 1.16 (tPAD) vs. 1.14 (LC Star), the Aw distribution tended to be less for the tPAD vs. LC Star, 9.7 vs. 21.9% respectively ($p = 0.22$). LargeAw distribution was significantly less for the tPAD vs. LC Star, 2.4 vs. 12.5%, as was Large/InterAw, 2.6 vs. 13.3% respectively ($p < 0.05$ by Wilcoxon signed-rank test). SmallAw distribution was similar between the two devices, 7 (tPAD) and 8.5 (LC Star) %.

Conclusions: The distribution of inhaled aerosol deposition via the tPAD and LC Star appeared to be equivalent using standard deposition measures, e.g., % lung deposition and C/P ratio. However, using measurements of clearance for the deposited insoluble, radiolabeled particles we were able to discern clear differences in regional deposition within large and intermediate airways between the two devices. Such clearance measurements should be considered to provide better resolution for regional deposition of nebulized, aerosolized drug delivery. Supported by NIH P01 HL108808 and Parion Sciences, Inc.

1MD.3

Improved Prediction Of Intersubject Variability In Extrathoracic Aerosol Deposition. Conor A. Ruzycki, Michael Yang, Scott Tavernini, C. Paul Moore, Michelle L. Noga, Andrew R. Martin, Hak-Kim Chan, WARREN H. FINLAY, *University of Alberta*

Orally inhaled aerosols must pass through the extrathoracic region in order to deposit in the lungs. Variability in extrathoracic deposition between different subjects thus leads to variability in the dose delivered to the lungs. The ability to predict such intersubject variability is useful both for risk exposure assessment with inhaled environmental aerosols, as well as in the development of medical aerosol products. Traditional algebraic correlations that were first developed for radiological protection models have been used to predict intersubject variability in extrathoracic deposition. However, these correlations have recently been found to significantly underpredict intersubject variability in mouth-throat deposition. In order to provide more accurate estimates of intersubject variability, we have made use of in vitro data in which we have measured extrathoracic deposition in realistic replicas of the extrathoracic airways of several dozen subjects ranging in age from newborn infants to adults. From this dataset, a theoretical analysis based on uncertainty propagation was developed in order to predict in vivo intersubject variability. To examine the accuracy of these predictions, in vivo measurements of mouth-throat deposition in adults inhaling aerosol during tidal breathing were performed on an independent set of subjects using SPECT scintigraphy. Intersubject variability was found to be in good agreement with our predicted values. For a given aerosol, intersubject variability in extrathoracic deposition is caused by intersubject variations in inhalation flow rate, intersubject variations in geometry captured by a characteristic extrathoracic airway diameter d_c, and intersubject variations caused by geometrical differences in the extrathoracic airways that are not captured by d_c (i.e. geometric dissimilarity). All three factors are found to play a role in causing intersubject variability. The presented methods may be useful to those wanting to predict, understand and control the sources of extrathoracic intersubject variability with inhaled aerosols.

1MD.4

Phenotyping of Chronic Obstructive Disease, COPD, from Deposition Fractions of Inhaled Nanoparticles. JAKOB LÖNDAHL, Jonas Jakobsson, H Laura Aaltonen, Eeva Piitulainen, Per Wollmer, *Lund University, Sweeden*

COPD is one of our most common diseases, globally causing about three million deaths each year and an economic loss of more than two trillion USD. The disease is characterized by poor airflow and shortness of breath, often resulting from smoking or long-term exposure to air pollution. Two major phenotypes of COPD are predominantly bronchial disease with narrowing of the conducting airways, and emphysema, which is damage and enlargement of the terminal airways including the alveoli. A precise diagnosis is important for treatment, but currently there is a lack of cheap and specific methods to diagnose COPD – especially in the form of emphysema.

We have previously suggested that inhaled nanoparticles can be used as a probe to assess dimensions of the small airspaces in the lung (Löndahl et al. 2017). The method, named Airspace Dimension Assessment (AiDA), derives dimensions of the peripheral airspaces from the half-life time of airborne nanoparticles. Enlarged airspaces result in a decreased deposition and hence a longer half-life. The objective of this study was to investigate if AiDA can provide information about emphysema.

AiDA measurements were carried out on 66 subjects: 25 healthy, 23 smokers with COPD and 18 subjects with alpha-1 antitrypsin deficiency (AATD). AATD is a genetic disorder that greatly increases the risk to develop emphysema. This group differs from smokers with COPD, which are likely to have both bronchial disease and emphysema. A comprehensive investigation of lung function was carried out for all subjects, including spirometry, diffusion capacity of the lung for carbon monoxide ($D_{L,CO}$) and forced oscillation technique (FOT). Computed tomography (CT) scans of the chest were made for the smokers and the AATD group.

An instrument for deposition measurements of nanoparticles has been developed as described in detail elsewhere (Jakobsson et al. 2017). Measurements were carried out with 50 nm particles sampled from a volumetric lung depth of 1100-1300 ml after a single breath-hold. To obtain the half-life time of the particles, six measurements were performed for each subject with breath-holds varying between 5-10 s. Data were aggregated into two numbers: an airspace dimension calculated from the nanoparticle half-life and a parameter named intercept, which is related to particle losses in the conducting airways.

In a first analysis of the data, the peripheral airspace dimensions derived from AiDA were 0.27±0.03 mm, 0.37±0.07 mm and 0.34±0.08 mm for healthy, smokers and AATD subjects, respectively. Both groups with disease differed significantly from the healthy subjects ($p<0.001$), which indicate presence of emphysema. The AiDA intercept was 0.50±0.18, 0.33±0.18 and 0.50±0.22, for the three groups: healthy, smokers and AATD. Thus, the AATD group had almost identical intercept as the healthy subjects, while the smokers deviated significantly ($p<0.01$), which imply that the smokers, but not the AATD group, had changes in the conducting airways compared to the healthy subjects. AiDA data correlated significantly with measures of emphysema from $D_{L,CO}$ and CT.

In conclusion, this study shows that AiDA has potential as a new method for detection and phenotyping of lung disease. The method is less expensive than CT and does not involve radiation. It is more specific to lung geometry than $D_{L,CO}$ and is in no need of pressurized CO. Thus, it has ability to be more widely available in healthcare, which would facilitate early discovery of COPD.

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1MD.5

Validating CFD Predictions of Small Particle Aerosol Deposition in a Infant Nasal Airway Model. KARL BASS, Susan Boc, Michael Hindle, Worth Longest, *Virginia Commonwealth University*

Nose-to-lung (N2L) administration of enhanced excipient growth (EEG) particles or droplets is expected to increase lung dose and improve targeted delivery of treatments for infants with respiratory diseases, such as Cystic Fibrosis (CF) and Respiratory Syncytial Virus (RSV). With EEG delivery, small particles or droplets (<2µm) enter the nasal cavity via a streamlined nasal cannula and are able to penetrate to the lower airways due to decreased impaction deposition. The hygroscopic excipient of these particles/droplets allows them to absorb moisture in the humid airway conditions and hence increase in diameter, which leads to increased deposition deep in the lungs. The use of CFD and in vitro models has proven a valuable tool to progress the development of the condensational growth approaches for pharmaceutical aerosol delivery. The CFD model must be validated against experimental data to ensure accuracy of the numerical results, and provides greater insight into the transport physics and particle/droplet deposition sites. The objective of this study was to validate mesh and solution parameters against experimental data for accurate modelling of microparticle deposition in an infant nasal airway for the assessment of N2L aerosol administration. The infant nasal model was generated by segmentation of CT scans in the Mimics and 3-matic software packages, and a CAD model developed in SolidWorks. The scan was chosen from an in-house database using selection criteria that are representative of a six-month-old infant: height and weight were between the 25th and 75th percentile, the mouth was closed as is typical during nasal drug administration, and the scan resolution was sufficient to build an accurate model. A Stratasys Objet 24 3D printer was used to build the experimental model, which included connections for the streamlined nasal cannula and outlet filter. A set of CFD meshing and solution guidelines, which were previously developed by our group for aerosol deposition in low Reynolds number and transitional turbulence, were applied to the CFD model in an effort to ensure accurate and reliable results. The CFD model was meshed and transport equations were solved using the capabilities provided by the ANSYS software suite of products with additional in-house user codes to address near-wall turbulence and particle-wall interactions. Comparisons are made between different meshing strategies, such as tetrahedral, cut-cell, and polyhedral cells, mono- and poly-disperse particle size distributions, and laminar or k-omega flow models. Furthermore, a wall roughness model is included to evaluate its accuracy compared to experimental pressure drop, and the effect on the near-wall velocity and turbulence fields. Application of predetermined CFD model guidelines provided results that compared well with experimental deposition data. The results also demonstrate that the two-equation k-omega model is capable of accurately capturing microparticle deposition, without the need for more complex turbulence models. As expected, the low nasal deposition of small EEG particles leads to high lung dose, with more that 90% of particles exiting the experimental and CFD model outlet. This study provides further validation of our previously developed meshing and solution guidelines, with good comparisons drawn between CFD and experimental deposition data in the complexities of an infant nasal model. The CFD model also utilized the wall roughness model, which provides a more realistic representation of the physical characteristics of the in vitro model wall surfaces, and is known to influence the skin friction, pressure drop, and near-wall flow field. For medical applications, the particle deposition data shows that the N2L EEG approach to aerosol delivery provides a highly efficient and targeted method of respiratory drug delivery to infants.

1MD.6

Intranasal and Tracheal Deposition of Dry Particles in 3D Physical Models of Rhesus Macaques. JANA KESAVAN, Valerie J. Alstadt, Jerold Bottiger, Beth Laube, *US ARMY ECBC*

Background: Quantification of particle deposition in the respiratory system of animals is used to assess environmental exposures and the effectiveness of drug delivery. In particular, assessments of toxicological agents and vaccine delivery are often conducted in rhesus macaques and the results are extrapolated to humans. Since rhesus macaques are obligate nose-breathers, it is important to know the percentage of inhaled particles that is lost to deposition in the intranasal airways and trachea and the percentage that is available for delivery to the lungs to make accurate exposure assessments. However, little is known of intranasal and tracheal deposition in rhesus macaques and less is known about dry power deposition in these animals, since most studies are conducted with liquid particles and do not quantify intranasal and tracheal deposition. Because the approval process is long and testing is expensive in live animals, we chose to address this information gap using 3D-printed, anatomically-correct models of rhesus macaques. Methods: Five models were generated from the CT scans of the head and trachea of four female macaques and one male macaque, using 3D-printing technology. The monkeys ranged in age from 3-9 years of age. The models contained the intranasal region (i.e. nasal passage, pharynx, larynx) and the trachea. Deposition fraction was determined using solid polydispersed Arizona Test Dust (ATD) aerosols that contained dry particles ranging in size between 0.5 to 10 microns. Models were individually placed in a chamber and were connected to a vacuum pump that pulled a constant airflow at 2, 4 or 6 L/min through the model. An Aerodynamic Particle Sizer (APS) was used to measure the particle size and the concentration of the test aerosol that entered the nose (upstream aerosol concentration) and exited the trachea (downstream concentration). Approximately 0.06 g of ATD was aerosolized into the chamber and the air was mixed for 45 seconds to obtain uniform aerosol concentration in the chamber. The APS sampled the upstream and downstream aerosol concentrations for 20 seconds. Deposition fraction was calculated for each run by dividing the downstream measurement by the average of the preceding and following upstream measurements. Deposition fraction was expressed as a combination of deposition in the intranasal and tracheal regions. Deposition fraction was plotted as a function of particle size and impaction parameter (diameter squared multiplied by air flow rate). Results: Deposition fraction in the intranasal and tracheal regions combined increased as particle size and/or air flow rate increased and as the impaction parameter increased. Three of the models had similar deposition curves, whereas the other two models had higher deposition curves when the data were plotted as a function of impaction parameter. Deposition efficiency curves for three of the models indicated only 10% deposition for the impaction parameter of 1000 µm2 cm3 s-1. Deposition efficiency curves for the other two models showed approximately 50% and 65% deposition for the same impaction parameter. Conclusions: These findings indicate there was significant variability in the deposition of dry particles in the intranasal and tracheal regions of the 3D-printed models of these rhesus macaques. Such variability suggests there could be significant differences in dry particle deposition in the lungs of these animals as well, which differences could ultimately affect individual animal responses to toxic and therapeutic agents, thereby affecting interpretation of the data. Additional studies using this model approach could provide much needed information about deposition of dry particles in the intranasal and tracheal regions of rhesus macaques, which could lead to more accurate interpretations of toxic and therapeutic environmental exposures, without exposing the animal to the inhaled agents.

1MD.7

In Vitro Determination of Combivent and Spiriva Respimat Dose Delivery in Simulated Spontaneously Breathing Tracheostomy Patients. RYM MEHRI, Abubakar Alatrash, Edgar A. Matida, Fiorenza Frank, *Carleton University, Ottawa, ON, Canada*

Chronic obstructive pulmonary disease (COPD) is a common lung disease that affects the respiratory tract by obstructing the airflow from the lung, hence causing breathing difficulties. Aerosols are commonly used to deliver therapeutic drugs to patient suffering from asthma and COPD. The Spiriva Respimat Soft Mist Inhaler (SMI, Boehringer Ingelheim, Ingelheim, Germany) is capable of delivering a metered dose of aqueous medication (2.5 mcg of tiotropium bromide monohydrate/puff) in the form of aerosols, used in the treatment of COPD. The Respimat SMI is a new generation of inhaler, which generates an aerosol mist suitable for inhalation using mechanical power from a spring in comparison to the liquid-gas propellant typically used in pMDIs. This inhaler was designed to deliver a slow (initial approximate droplet velocity of 10 m/s) but lasting (approximately 1.5 seconds) aerosol mist to facilitate the coordination of actuation with inhalation for proper medication delivery. The inhaled drug efficiency is strongly influenced by the amount of inhaled drug, the aerosol characteristics (particle size distribution), the deposited mass, the delivery method, the flow characteristics and the architecture of airways. For patients with acute or severe COPD, mechanical ventilation is necessary to reduce the patient's work of breathing. In severe cases (unconscious patients), invasive mechanical ventilation is performed using tracheostomy or endotracheal tube, while simultaneously delivering medication. However, the Respimat SMI is not specifically designed to be used in intensive care, greatly affecting the inhaled drug deposition when using mechanical ventilation for patients with tracheostomy or endotracheal tube.

The purpose of this work is to study the aerosol particle deposition, in an experimental set up (in vitro), using a trachea replica (rapid prototyping). The set up attempts to replicate clinical setting for mechanically ventilated patients with COPD via tracheostomy tube. Tiotropium bromide monohydrate is delivered using the Respimat SMI via a spring loaded T-piece connected to an adapter (ODAPT). The ODAPT adapter was previously tested experimentally in continuous flow and using a mechanical ventilator to determine the effect of the adapter and T-piece on medication losses. Using these results, it is possible to properly estimate the medication lost in the ODAPT adapter and T-piece used in the experimental set up.

1MD.8

Human Nasal Olfactory Deposition of Inhaled Nanoparticles. LIN TIAN, Yidan Shang, Jingliang Dong, Kiao Inthavong, Jiyuan Tu, *RMIT University*

Olfactory pathway, susceptible for direct translocation of inhaled nanoparticles into the brain, has been verified in a number of animal studies. The extremely low dose toxic substance strongly suggests subclinical condition that prevents noticeable neurodegeneration until years after prolonged exposure. The exact mechanism, between elevated presence of toxic substances (e.g. heavy metals) and deteriorated neurofunction in human central nervous system, is still not clear; however, nasal olfactory, being portal of the entry for such a transport route, is undoubtedly a critical junction where hint to the time course and dose dependency might be inferred. Using a physiologically realistic nasal and upper airway replica, this study performed human inhalation simulations of nanoparticles (1 to 100 nm) under low to moderate breathing conditions (5 to 14 L/min). Olfactory deposition and the various factors contributing to the process were evaluated. Details on airflow pattern and particle flux in nasal and olfactory were made visible using a 2D unwrapped surface mapping technique, and it was found out that airflow pattern, especially nasal wall shear had a remarkable correlation to particle movement and deposition at the ultrafine scale (< 1~2 nm). Olfactory deposition efficiency was found to be extremely low (< 3.5%), and showed distinctive variation in high diffusivity region when compared to that in the entire nasal cavity. The entrance profile of olfactory deposited particles was seen to be highly selective and unanimously originated from upper section of the nostril near nasal septum. Current study is of significant value to the understanding of human uptake of inhaled nanoparticles through olfactory pathway.

1OF.1

Chlorine and Nitrate Radical Generation in Oxidation Flow Reactors. ANDREW LAMBE, Jordan Krechmer, Ezra Wood, William Brune, Douglas Worsnop, *Aerodyne Research, Inc.*

The majority of oxidation flow reactor (OFR) applications to date involve the generation of hydroxyl (OH) radicals to study daytime multigenerational oxidation of secondary organic aerosol (SOA) precursors. Other atmospheric radicals may also initiate SOA formation, with their relative importance dependent on the specific source region and radical precursor diel profile. Here, we present results from experiments using novel techniques to generate chlorine (Cl) and nitrate (NO_3) radicals in the Aerodyne Potential Aerosol Mass OFR for the study of polluted marine and nighttime source regions, respectively. We provide experimental and model evaluation of Cl and NO_3 generation capabilities as a function of OFR operating conditions. We use proton transfer reaction and chemical ionization mass spectrometer measurements to characterize precursors and oxidation products generated from the Cl and NO_3 oxidation of representative SOA precursors. Finally, we discuss the combined use of OH, Cl and NO_3 radicals to (1) evaluate the fate of known SOA precursors under different atmospheric conditions and (2) constrain the composition of unknown SOA precursors with different OH, Cl and NO_3-initated oxidation rates and SOA formation potentials.

1OF.2

Organic Peroxy Chemistry in Oxidation Flow Reactors and Chambers and Their Atmospheric Relevance. ZHE PENG, Julia Lee-Taylor, John Orlando, Geoffrey Tyndall, Jose-Luis Jimenez, *University of Colorado-Boulder*

Oxidation flow reactors (OFR) are a promising alternative to environmental chambers for investigating atmospheric oxidation processes and secondary aerosol formation. Because of their portability, short residence times, and ability to reach high photochemical ages, they have been increasingly employed in both lab and field studies. However, questions have been raised about how representative the chemistry within OFRs is of that in the troposphere. We investigate the fates of organic peroxy radicals (RO_2), which play a central role in atmospheric organic chemistry, in OFRs, environmental chambers, and under ambient conditions by chemical kinetic modeling. We simulate RO_2 fate in OFRs over a wide range of conditions (both low-NO and high-NO) and compare the results with RO_2 fates in key chamber and atmospheric conditions. For most types of RO_2, their bimolecular fate is mainly RO_2+HO_2 and RO_2+NO, similar to those in chambers and the atmospheric studies. For α,β-substituted primary (SPRO2) and acyl RO_2 (aRO2), RO_2+RO_2 can be significant in RO_2 fate. However, the relative importance of RO_2+RO_2 is sensitive to HO_x recycling ratio of the reaction system. At our best estimate of HO_x recycling ratio (~0.3), RO_2+RO_2 can be the most important bimolecular loss pathway of SPRO2 and aRO2, but still can generally cover the range of the relative importance of RO_2+RO_2 of SPRO2 and aRO2 in chambers and the atmosphere. This is can be explained by HO_2 increased together with OH in OFRs. The OH-to-HO_2 ratio in OFRs covers the ambient values (on the order of 0.01), but can be significantly higher (on the order of 0.1) at high water vapor concentrations, high UV settings, and low precursor concentrations. A low-NO OFR experiments under these conditions could lead to substantial relative contribution of recently proposed, but highly uncertain RO_2+OH to RO_2 fate, much higher than the highest ambient value (~10%). For aRO2, if they do not undergo very fast isomerization in OFRs, they would be substantially (even dominantly) consumed by NO_2 as long as significant amounts of NO precursor(s) are injected into OFRs. $RO_2+NO_2 \rightarrow RO_2NO_2$ is not a sink of aRO2 in chambers and the atmosphere, but it is a sink in OFRs, where the thermal decomposition lifetimes of the product, peroxynitrates (hours), is longer than OFR residence times (minutes). Short residence times of OFRs also prevent RO_2 isomerization in OFRs from proceeding to the same extent as in the atmosphere. Nevertheless, as long as the isomerization of an RO_2 is important in the atmosphere, this isomerization is significant in OFRs, and far from negligible as some researchers have speculated. Overall, chambers generally can obtain atmospherically relevant RO_2 fates; so can OFRs to a large extent. Most importantly, careful attention to OFR (and chamber) operating conditions needs to be paid to simulate specific RO_2 fates, such as avoiding atmospherically irrelevant organic photolysis when increasing VOC concentrations to achieve higher RO_2+RO_2 and/or NO precursor concentrations to achieve higher RO_2+NO.

1OF.3

Modeling the Formation and Composition of Secondary Organic Aerosol in Oxidation Flow Reactors Using Simple and Detailed Chemistry and Thermodynamic Models. Sailaja Eluri, Christopher Cappa, Beth Friedman, Delphine Farmer, SHANTANU JATHAR, *Colorado State University*

Oxidation flow reactors (OFRs) are being increasingly used to study the photochemical production of secondary organic aerosol from both anthropogenic and natural sources. Compared to environmental chambers, OFRs are smaller, easier to operate, allow for much longer photochemical exposures, and are less susceptible to gas and particle wall losses. Yet, there are concerns that high oxidant concentrations and kinetic limitations to gas/particle partitioning may affect the formation and composition of SOA in OFRs. Hence, there is a need to develop and use modeling tools to interpret OFR data and facilitate translation of OFR results to the real atmosphere.

Recently our group reported on experiments that used an OFR to measure the photochemical production of SOA from a diesel engine operated at two different engine loads (idle, load), two fuel types (diesel, biodiesel) and two aftertreatment configurations (with and without an oxidation catalyst and particle filter). In this work, we used two different SOA models, the volatility basis set (VBS) model and the statistical oxidation model (SOM), to simulate the formation and composition of SOA for those experiments. Leveraging recent laboratory-based parameterizations, both frameworks accounted for a semi-volatile and reactive POA; SOA production from semi-volatile, intermediate-volatility and volatile organic compounds (SVOC, IVOC and VOC); multigenerational gas-phase chemistry; and kinetic gas/particle partitioning. Both models suggested that for model predictions of SOA mass to agree with measurements across all engine load-fuel-aftertreatment combinations, it was necessary to model the kinetically-limited gas-particle partitioning in OFRs as well as account for SOA formation from IVOCs. IVOCs were found to account for more than 90% of the model-predicted SOA but accounting for them resulted in an under-prediction of a factor of two for OA atomic oxygen-to-carbon ratios. Model predictions of the gas-phase organic compounds, resolved in carbon and oxygen space, from the SOM compared favorably to gas-phase measurements from a Chemical Ionization Mass Spectrometer (CIMS), substantiating the semi-explicit chemistry captured by the SOM. Model-measurement comparisons were improved on using vapor wall-loss corrected SOA parameterizations but remained insensitive to OFR-specific parameters such as residence time distributions and spatial heterogeneity in oxidant concentrations.

As OFRs are increasingly used to study SOA formation and evolution in laboratory and field environments, models such as those developed in this work can be used to interpret OFR data.

1OF.4

Aging of Selected Particulate Organic Markers in Oxidation Flow Reactors. LIN WANG, Mingyi Wang, Lei Yao, Hangfei Chen, Bowen Zhang, Xiaoyu Hu, *Fudan University*

Aging of organic aerosol particles is one of the least understood topics in atmospheric aerosol research. Here, we used self-made oxidation flow tubes at laminar flow conditions to study OH radical or ozone-initiated aging of selected particulate organic markers, including oleic acid, squalane, and squalene. Pure organic particles were generated via homogeneous nucleation by passing an ultrahigh purity nitrogen over an insulated organic standard and subsequent diluting with zero air. Ozone was produced by photolysis of molecular oxygen using a Hg pen-ray lamp, and OH radical was produced by passing a mixed flow of ozone and water vapor through 254 nm light. We examined gaseous and particulate products by a high-resolution time-of-flight chemical ionization mass spectrometer equipped with a Filter Inlet for Gases and AEROsols (FIGAERO-HRToF-CIMS) using the iodide ion (I-) as the reagent ion. Our results indicate that ozonolysis of an unsaturated particulate species is characterized with formation of high-molecular-weight particulate products through reactions of stabilized Criegee intermediates. On the other hand, OH radical-initiated reactions are featured with multiple reaction mechanisms, especially fragmentation and isomization of the main carbon chain. Our study clearly demonstrates the complexity of atmospheric heterogeneous reactions. A detailed understanding of these mechanisms permits accurate treatment of heterogeneous aging processes in global models in order to better understand the evolution of organic aerosols and to constrain their physicochemical properties including carbon oxidation state, hygroscopicity, and CCN activity throughout their atmospheric lifetime.

1OF.5

A Perspective on Developing “Wall-less” Oxidation Flow Reactors. WILLIAM BRUNE, Andrew Lambe, *Pennsylvania State University*

Environmental chambers and oxidation flow reactors (OFRs) enable the controlled experiments on secondary aerosol (SA) chemistry that are almost never possible in the atmosphere. The experiments provide models with essential quantitative numerical properties such as secondary aerosol nucleation rates, mass yields, chemical composition, hygroscopicity, and optical properties. Unfortunately, the walls of environmental chambers and OFRs can contaminate these experimental results by interacting with the gas-phase and particle-phase chemistry and microphysics. In this presentation, we describe a way to think about developing “wall-less” OFRs and show how the optimal design of each OFR depends on the range of environmental conditions and SA properties to be studied. We provide examples of novel OFR designs and demonstrate the suppression of wall effects compared to conventional OFRs and environmental chambers.

1OF.6

Characterizing Photochemical Environment in the Caltech PhotoOxidation Flow Tube Reactor (CPOT). YUANLONG HUANG, Ran Zhao, John Seinfeld, *California Institute of Technology*

Flow tube reactors have been widely employed to study gas-phase atmospheric chemistry and secondary organic aerosol (SOA) formation. The Caltech PhotoOxidation flow Tube (CPOT) reactor is designed to investigate SOA related gas- and particle- phase photochemical reactions. Hydrogen peroxide serves as the source of hydroxyl radical (OH) under UV radiation. We report here the characterization of the photochemical environment in the CPOT through both experimental and modeling studies. Emphasis will be placed on the influence of the OH-wall interaction and the external OH reactivity (determined with sulfur dioxide and volatile organic compounds) on the photooxidative capacity of the CPOT. We will also present a flow-pattern based method to incorporate the residence time distribution (RTD), which reflects the fluid mechanical non-ideality of the reactor, into both data interpretation and model simulation.

1OF.7

Secondary Aerosol from Gas Emissions of Sage (SAGES): Characterizing SOA Production from Coastal Sage Scrub Plant Emissions under High and Low NOx Conditions. CELIA FAIOLA, Chinmoy Sarkar, Jordan Krechmer, Archit Mehra, Leah Williams, Fatemeh Khalaj, Manjula Canagaratna, Alex Guenther, Dasa Gu, Arin Boghoz, Angelo Calinga, John Jayne, Douglas Worsnop, Andrew Lambe, *University of California Irvine*

Plants emit more than 1,700 different volatile compounds, but very few of these compounds have been the subject of systematic SOA laboratory studies. It is unclear if a complex mixture of plant volatiles will generate SOA in a predictable way based on a linear combination of the individual components. Furthermore, it is unclear if the handful of proxy compounds that have been used in most SOA lab studies adequately represent the SOA chemistry of real plant emissions containing unique compounds that have not been studied previously. Thus, there are two major gaps in SOA studies: 1) investigations of realistic complex VOC mixtures and 2) investigations of plant volatiles that have not been the subject of previous lab studies. We addressed these two critical gaps by exposure of Salvia mellifera (black sage) and Artemisia californica (california sagebrush) emissions to O3, OH, and NO3 in the Aerodyne Potential Aerosol Mass oxidation flow reactor. These plants are keystone species in the Southern California coastal sage scrub ecosystem. SOA production was observed via OH exposure under low- and high-NO conditions, but not via O3 or NO3 exposure. The plant emissions and ensuing SOA formation were dominated by compounds that have not been targeted in previous SOA studies, including oxygenated monoterpenes such as camphor, 1,8-cineole, and alpha-thujone. For comparison to the mixture, these three compounds that dominated emissions from black sage were individually exposed to OH radicals. Gas-phase emissions were characterized with GC-ToF-MS and a Vocus PTR-MS, which also measured oxidized products. Particle size distributions and composition were characterized with a scanning mobility particle sizer and an HR-LToF-AMS. An overview of the experiments will be presented including detailed plant emission profiles, SOA yields, and SOA composition.

1OF.8

Real-time and Off-line Applications of Oxidative Flow Reactor (OFR) for Chemical and Physical Characterization of Secondary Organic Aerosols (SOA). YONG JIE LI, Pengfei Liu, Qi Chen, Yan Zheng, Xi Cheng, Keren Liao, Scot T. Martin, *University of Macau*

Secondary organic aerosols (SOA) are major components in atmospheric particulate organic matters. The chemical and physical properties, as well as their dynamic evolution, are crucial in our understanding of the impacts of SOA. Fundamental investigations on SOA are usually done with large-scale smog chamber facilities (SCF) or small-scale oxidative flow reactors (OFR). The flexibility of OFR makes it an attractive alternative to SCF for SOA studies. Lab-based or field-based OFR studies have offered new insights in SOA from a variety of precursors (Lambe, et al., 2011, Lambe, et al., 2012) and in different environments (Hu, et al., 2016, Palm, et al., 2018) using real-time characterization. Apart from real-time approaches, sampling of SOA after OFR for off-line analysis or processing can also be used to study different aspects of SOA properties. We will present applications of OFR for characterization of SOA using both real-time and off-line approaches. Physical and chemical characteristics of SOA from different precursors were obtained before and after exposure to gaseous ammonia to study the effects of phase state on SOA reactivity (Li, et al., 2015). A lot more characterization can be applied to SOA samples collected by either conventional filter sampling and/or thin-film formation using an electrostatic precipitator (Liu, et al., 2013). SOA collected on an attenuation total reflection (ATR) crystal aged with ammonia was investigated with Fourier transfer infrared (FTIR) spectroscopy; browning of SOA by ammonia was studied with UV-vis spectrometry (Liu, et al., 2018); evaporation kinetics and hygroscopicity were measured for the SOA film using a quartz crystal microbalance (QCM) (Liu, et al., 2016, Liu, et al., 2018). To extend these real-time and off-line applications of OFR in high-NOx conditions commonly found in urban environments, OH exposure calibration results for OFR185 and OFR254 with or without N2O injection will also be presented.

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1RA.1

Measured Contributions to Cloud Condensation Nuclei from DMS and Sea Spray in the Marine Atmosphere. Kevin Sanchez, Chia-Li Chen, LYNN RUSSELL, Raghu Betha, Jun Liu, Derek Price, Paola Massoli, Luke Ziemba, Ewan Crosbie, Richard Moore, Markus Müller, Sven A. Schiller, Armin Wisthaler, Alex Lee, Patricia Quinn, Timothy Bates, Jack Porter, Thomas Bell, Eric Saltzmann, Robert D. Vaillancourt, Michael Behrenfeld, *Scripps Institution of Oceanography*

Biogenic sources contribute to cloud condensation nuclei (CCN) in the clean marine atmosphere, but few measurements exist to constrain climate model simulations of their importance. The chemical composition of individual atmospheric aerosol particles showed two types of sulfate-containing particles in clean marine air masses in addition to mass-based Estimated Salt particles. Both types of sulfate particles lack combustion tracers and correlate, for some conditions to atmospheric or seawater dimethyl sulfide (DMS) concentrations, which means their source was largely biogenic. The first type is identified as New Sulfate because their large sulfate mass fraction (63% sulfate) and association with entrainment conditions means they could have formed by nucleation in the free troposphere. The second type is Added Sulfate particles (38% sulfate), because they are preexisting particles onto which additional sulfate condensed. New Sulfate particles accounted for 31% (7 cm-3) and 33% (36 cm-3) CCN at 0.1% supersaturation in late-autumn and late-spring, respectively, whereas sea spray provided 55% (13 cm-3) in late-autumn but only 4% (4 cm-3) in late-spring. Our results show a clear seasonal difference in the marine CCN budget, which illustrate how important phytoplankton-produced DMS emissions are for CCN in the North Atlantic.

1RA.2

South African Biomass Burning Season Aerosols Observed over the Remote Southeast Atlantic Ocean on Ascension Island. Allison Aiken, Paquita Zuidema, Arthur J. Sedlacek, THOMAS WATSON, Stephen Springston, Connor Flynn, Chongai Kuang, Janek Uin, Manvendra Dubey, *Los Alamos National Lab*

Biomass burning (BB) emissions are a large source of carbon to the atmosphere via particles and gas phase species. With a potential rise in drought and extreme events in the future, these numbers are expected to increase. From approximately June-October every year, the plume of South African BB emissions, the largest BB source in the world, are advected west and are known to impact both the boundary layer and free troposphere at Ascension Island (Zuidema et al., 2016). Ascension Island is located 8 degrees South of the Equator and 15 degrees West Longitude in the middle of the South Atlantic Ocean, at least 1000 miles from any major shoreline and closest to the continent of Africa. During the U.S. DOE ARM field campaign, Layered Atlantic Smoke Interactions with Clouds (LASIC), direct online in situ measurements of aerosol and trace gases were collected continuously on Ascension Island from June 2016 through October 2017 spanning a ~1.5 year period. While low Southern Hemisphere background aerosol and trace gas measurements are observed most of the year that picture changes during the South African BB season.

Two BB seasons are contrasted with the near pristine background conditions during the campaign from the ARM Aerosol Mobile Facility 1 (AMF1) and Mobile Aerosol Observing System (MAOS). Refractory light absorbing carbon mass concentrations reach 1 μg m-3 during multiday plumes and exceed 25% of the total aerosol submicron mass concentration, contrasting significantly with BB plumes observed over the Southwestern United States (SW US) and South America (Brazil). Numerous direct in situ aerosol and trace gas measurements are presented, e.g. submicron non-refractory chemical composition (Organics, Sulfate, Nitrate, Ammonium, Chloride), refractory soot, PM1 and PM10 aerosol absorption and scattering, carbon monoxide (CO), etc. Aerosol and trace gas signatures are investigated along with backtrajectories to identify sources. Carbonaceous aerosols emitted with gas-phase CO are used to determine particulate emission ratios along with intrinsic and extrinsic aerosol properties.

Comparison will be made between the aerosol species observed during LASIC versus BB from wildfires measured in the SW US and Brazil. Results from single fuel laboratory studies probed with aerosol mass spectrometry alongside aerosol optical properties will also be presented contrasting near source and far field BB emission profiles. Organic Aerosol (OA) to refractory soot ratios of ~2.4 observed in the BB plumes from South Africa on Ascension Island are much higher than BB emissions sampled from forest fires in the SW US and BB sources in Brazil. The differences observed between BB emissions in different regions highlights the need to further understand the different atmospheric chemistries within the context of the differing background conditions in the two hemispheres, including differences in BB fuel types and combustion conditions.

1RA.3

Marine Boundary Layer Aerosol in Eastern North Atlantic: Seasonal Variations and the Key Controlling Processes.

GUANGJIE ZHENG, Tamara Pinterich, Allison Aiken, Robert Bullard, Edward Luke, Pavlos Kollias, Chongai Kuang, Stephen Springston, Janek Uin, Thomas Watson, Rob Wood, Jian Wang, *Brookhaven National Laboratory*

The response of marine low cloud systems to changes in aerosols represents one of the largest uncertainties in climate simulations. Major contributions to this uncertainty derive from poor understanding of aerosol under natural conditions and the perturbation by anthropogenic emissions. The Eastern North Atlantic Ocean (ENA) is a region of persistent but diverse marine boundary layer (MBL) clouds, and whose albedo and precipitation are highly susceptible to perturbation in aerosol properties. In this study, we examine aerosol properties, trace gas concentrations, and meteorological parameters measured at the ARM ENA site on Graciosa Island since 2014. Aerosol size distribution from 55 nm to 1 µm typically consists of three modes: Aitken (At), Accumulation (Ac) and Sea Spray Aerosol (SSA) modes. Observed CCN number concentrations are in general agreement with the sum of Ac and SSA mode concentrations. The number concentration of SSA mode, mainly driven by sea spray aerosol (SSA) production and precipitation scavenging, is higher in winter and lower during summer. The entrainment of free tropospheric aerosols, including long range transported continental pollution, represents a major source of At and Ac mode particles. In comparison, SSA often contributes to a minor fraction of At and Ac mode number concentrations, with estimated mean annual contribution around 4.5% and 21%, respectively. For the combined population of At and Ac mode particles, coalescence scavenging represents the major sink, while coagulation of At mode particles with Ac and SSA mode particles and activated droplets inside clouds can also play a role. Higher contribution of entrained free tropospheric aerosol is coincident with stronger precipitation during spring and winter seasons. As a result, At and Ac mode number concentrations exhibit weak seasonal variations, with slightly higher levels during the spring and summer seasons.

1RA.4

Free Tropospheric Aerosol characteristics over the North Eastern Atlantic Ocean and Its Relationship to the Marine Boundary Layer. BIRGIT WEHNER, Karine Chevalier, Silvia Henning, Kay Weinhold, Oliver Welz, Claudio Mazzoleni, Paulo Fialho, Simeon Schum, Stefano Viviani, Greg Roberts, *Leibniz-Institute for Tropospheric Research*

Networks for continuous ground based measurements of aerosol particles have been established over the last decade. However, most of the measurement sites are located on continental areas and are not representative of marine regions. Roughly, 70% of Earth's surface is covered by water and thus, the knowledge of climate-relevant parameters such as aerosols, clouds and radiation also in marine regions is of high importance to understand the global climate.

Although the marine boundary layer structure over the oceans is considered simpler compared to continental boundary layers, decoupled layers with several levels often characterize the stratification. This system is not well understood up to now, for cloudy as well for cloud-free situations.

The ACORES campaign (Azores stratoCumulus measurements Of Radiation, turbulEnce and aeroSols) has been performed in July 2017 in the Azores, in the Atlantic Ocean. The overarching goals of the project was the detailed study of the stratification of the marine boundary layer in terms of clouds and aerosol properties. Besides helicopter-borne vertical measurements, this study comprises also ground-based measurements at sea level (ARM site ENA) and in the free troposphere (UAc site OMP - Pico Mountain Observatory, 2225 m).

Aerosol Particle number size distribution measurements between 10 nm and 10 µm at both sites (ENA and OMP) have been performed using a Mobility Particle Sizer System (MPSS) and an Aerodynamic Particle Sizer (APS) over 3 weeks in July 2017. In addition, a mini cloud condensation nuclei counter (CCNc) has been operated in flow scanning mode at the OMP site. Furthermore, measurements of aerosol scattering and absorption coefficients (or black carbon, BC), as well as meteorological data, are available.

A number of ground-based aerosol and meteorological, as well as remote sensing data completed the measurements at ENA (https://www.arm.gov/capabilities/observatories/ena).

During this campaign, we measured for the first time on Pico Mountain, particle number size distributions down to 10 nm and CCN concentrations. The data have been investigated for special features, such as new particle formation or long range transport of polluted air masses. The summer 2017 was relatively clean compared to earlier years and the number concentration of larger particles (> 100 nm) has been relatively low, as confirmed by low BC concentrations. Only two periods with slightly increased BC values have been observed, but values were still below 40 ng m^{-3}.

The aerosol number concentrations have been relatively low over the whole period, while small plumes, obviously caused by local anthropogenic pollution, often influenced the ENA site.

During nighttime, Pico Mountain was five times inside a cloud, i.e. the relative humidity was 100% and particles larger than 50 nm, as well as CCN, were completely removed, while smaller particles were still detected as interstitial aerosol.

On one day out of three weeks, new particle formation on Pico was observed while there was no clear event visible at ENA.

On the majority of measurement days, the particle number size distribution at sea level consisted of two modes. Instead, the particles in the FT showed typically only one mode, but, contradictory to previous studies, this mode occured in the Aitken mode range (< 100 nm) but also above 100 nm, i.e., in the accumulation mode, originated probably from long-range transport.

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1RA.5

Molecular and Physical Characteristics of Aerosol at a Remote Marine Free Troposphere Site: Implications for Atmospheric Aging. SIMEON SCHUM, Bo Zhang, Katja Dzepina, Swarup China, Paulo Fialho, Claudio Mazzoleni, Lynn Mazzoleni, *Michigan Technological University*

Marine regions cover a large fraction of the Earth's surface. In these regions, long range transported aerosol can play a key role on the Earth radiative balance by interacting with clouds and solar radiation. However, free tropospheric aerosol over the ocean are not well characterized due to the challenges of sampling in these remote areas. We analyzed the molecular and physical characteristics of long-range transported aerosol samples collected at the Pico Mountain Observatory (38° 28′ 15′′ N; 28° 24′ 14′′ W, 2225 m above mean sea level) in the North Atlantic Ocean. The Observatory is located in the marine free troposphere on Pico Island in the Azores archipelago, making it an excellent site for the study of aged organic aerosol with minimal influence of local emission sources. Specific samples were selected for detailed molecular study based on (1) elevated organic carbon concentrations and (2) FLEXPART simulations with the goal to capture pollution events of different origins. Water-soluble organic aerosol extracts were then analyzed using ultrahigh resolution mass spectrometry ($R > 200{,}000$) in order to elucidate their molecular characteristics. Thousands of molecular formulas were assigned to each of the individual samples. On average ~60 % of the molecular formulas contained only carbon, hydrogen, and oxygen atoms (CHO), ~30 % contained nitrogen (CHNO), and ~10 % contained sulfur (CHOS). In general, samples transported through the free troposphere were less oxidized than those transported through the boundary layer. Despite their longer residence times, average oxygen to carbon (O/C) ratios of less than 0.5 were observed for the free tropospheric aerosol, compared to O/C ratios greater than 0.5 for those transported in the boundary layer. Using the extracted ambient temperature and relative humidity from the FLEXPART-GFS/FNL simulations, the phase state of the water-soluble organic aerosol molecular species was estimated for up to 5 days before sampling. The low temperature and relative humidity in the free troposphere predict a solid phase for the organic aerosol, which likely increased its resistance to oxidation. The specific molecular differences in the overall oxidation between the free tropospheric transported aerosol and the boundary layer transported aerosol are presented, as well as the potential for aqueous phase oxidation and differences in the aerosol phase state.

1RA.6

Aerosol Particle Size Distributions and Compositions over the Southern Ocean in the Austral Summer of 2017.

TAKUMA MIYAKAWA, Fumikazu Taketani, Masayuki Takigawa, Chunmao Zhu, Kazuhiko Matsumoto, Yutaka Tobo, Momoka Yoshizue, Yugo Kanaya, *Japan Agency for Marine-Earth Science and Technology*

Aerosol particles in the marine boundary layer are emitted from the ocean surface through the sea-spraying process. They can affect the cloud formation over the ocean, resulting in their significance in the Earth's radiative budget, because the ocean aerial coverage is high on the earth. Southern Ocean (SO) is a unique region with rich ecosystems and without anthropogenic and continental natural impacts especially in austral summer (e.g., McCoy et al., 2015). To the best of our knowledge, the measurements of aerosol particles over the Pacific Ocean sector of SO are sparse and critically needed for understanding the concentration levels of aerosols to assess the role of aerosols as cloud condensation nuclei (CCN) in this region.

We have conducted ship-borne aerosol measurements using our research vessel "*Mirai*" in a framework of the research cruise "Trans South Pacific Project" between Japan and Chili (December 27, 2016-March 28, 2017). This cruise consisted 4 legs. RV "*Mirai*" was deployed over the SO (from Punta Arenas, CHL to Auckland, NZ) during the third leg in the late austral summer of 2017 (February 10-March 3, 2017). We have performed in-situ measurements of size distributions of total and non-volatile (at 300ºC) aerosol particles using a scanning mobility particle sizer (SMPS, TSI, the combination of a differential mobility analyzer model 3080 and a condensation particle counter model 3010), black carbon aerosol using a single particle soot photometer (SP2, DMT), and fluorescent bioaerosol particle (FBAP) using a wideband integrated bioaerosol sensor (WIBS4A, DMT) on the experimental room located on the upper level of RV Mirai. In the third leg, we performed air sampling for the post analyses of chemical composition, morphology (microscopy), and ice nucleating particles.

During the cruise of third leg, air masses without continental impacts were successfully observed except selected periods. We here assume the major source of aerosols in the MBL is the surface of the SO. Our observation results indicated that aerosol particles had the bimodal size distributions over the SO, which is commonly found in the MBL in a plenty of previous studies (e.g., Hoppel et al., 1990). The minimum diameter among two modes, so called Hoppel minimum (D_{HO}), was around 70 nm on average, which can be used for estimating the supersaturation SS level in the cloud process with the assumed chemical composition (Hoppel et al., 1986). The estimated value of SS varied from 0.2-0.4% with the assumption of pure ammonium sulfate during the cruise. We will present the temporal variations of size-segregated aerosol concentrations, CCN-proxy (particles larger than D_{HO}, e.g., Clarke and Kapustin, 2010), volume-fraction-remaining (VFR) at 300ºC as a diagnosis of the sea-salt particle impacts, FBAP, and the chemical composition (organic carbon) to elucidate the atmospheric physics and chemistry of natural aerosols in this region.

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1RA.7

Seasonal Variability of Aerosol Optical and Physical Properties from the Eastern North Atlantic (ENA) Aerosol Observing System (AOS) during 2016 and 2017. FRANCESCA GALLO, Allison Aiken, Connor Flynn, Annette Koontz, Jian Wang, Guangjie Zheng, Stephen Springston, Chongai Kuang, Janek Uin, Eduardo Azevedo, Kim Nitschke, *Los Alamos National Lab*

In the present study we assess the seasonal variability of aerosol optical and physical properties at the Eastern North Atlantic (ENA) Atmospheric Radiation Measurement (ARM) Facility. The ENA site is located in the remote Azores archipelago and is subject to strong meteorological variability during the year. Consequently, aerosol composition and concentration are affected by these meteorological variations. Especially, the combination of midlatitude, tropical and extratropical cyclones and strong surface wind speeds affect the Region during the winter, leading to the formation of coarse mode aerosols (e.g. sea salt), meanwhile the subtropical Azores high pressure system and diminished surface wind speeds in the summer lead to the production of fine mode aerosols. Here we show the seasonal variability of aerosol absorption, scattering and extinction coefficients (B_{abs}, Bsca and Bext) and intensive aerosol properties of light absorption, scattering and extinction Angstrom exponents (AAE, SAE and EAE) and single scatter albedo (SSA) for submicron (PM_1) and sub-10 µm (PM_{10}) diameter size cuts during the years 2016 and 2017 at ENA. Data were obtained through continuous measurement with the Aerosol Observing System (AOS) equipped with a 3 wavelength Nephelometer (450, 550, 700 nm) and PSAP (464, 529, 648 nm). Results indicate a seasonal trend in the PM_1 and PM_{10} aerosol optical properties during the period of study with the exception of PM_{10} SSA (0.90 ± 0.09). Total aerosol B_{abs} is dominated by the PM_1 fraction throughout the year (~60% of the total B_{abs} due to the submicron) while B_{sca} is dominated by the supermicron species (~ 70% of the total B_{sca} due to the PM_{10}). However, both B_{abs} and B_{sca} are highest in the winter and lower in the summer ranging respectively from seasonal averages of 0.46 – 0.70 Mm^{-1} and 5.35 – 7.38 Mm^{-1} in PM_1 and 0.77 – 1.15 Mm^{-1} and 14.8 – 26.57 Mm-^{1} in PM_{10}. B_{ext} shows seasonal variability in the PM_{10} fraction (seasonal averages ranging from 12.71 – 19.65 Mm^{-1}). Intensive aerosol properties also indicate a seasonal trend: while AAE is highest in the winter (seasonal averages ranging from 0.85 – 1.09 in PM_1 and from 0.96 – 1.12 in PM_{10}), SAE is highest in the summer (seasonal averages ranging from 1.88 – 1.18 in PM_1 and from 0.39 – 0.89 in PM_{10}). Combination of AAE and SAE spectral variability in PM_1 reveals the dominance of small particle diameters in the summer and the presence of mixed absorption species, dominated by soot in the winter. Changes in both meteorological conditions and emission source through the year could explain these variations. This hypothesis is also supported by the evaluation of wind speed and direction and total aerosol number concentration. Future investigations concerning aerosol size distributions from the UHSAS and chemical composition from the ACSM at ENA will be used to support our findings.

1RA.8

Variations in Composition of Particles Sampled at Different Altitudes in the North Atlantic. DANIEL VEGHTE, Swarup China, Joseph Charnawskas, Daniel Bonanno, Johannes Weis, Ryan Moffet, Mary Gilles, Daniel Knopf, Jian Wang, Alexander Laskin, *Pacific Northwest National Laboratory*

Atmospheric particles collected at varying altitudes in the remote region of the Azores archipelago were characterized using chemical imaging techniques. The particle samples were collected during the Aerosol and Cloud Experiment in the Eastern North Atlantic (ACE-ENA) field study, onboard the ARM aerial facility platform (G-1 aircraft) and at the ground ENA supersite. The ground site collection allowed for size resolved collection of aerosol particles at sea level utilizing a multistage impactor while sampling aboard the aircraft employed a custom built time resolved aerosol collector. Multi-modal chemical imaging of particles was performed using complementary capabilities of electron microscopy and scanning transmission X-ray microscopy. Additionally, high resolution mass spectrometry was used to characterize the chemical composition of the organic fraction of collected particles. In additional experiments, collected particles were investigated by in-situ electron microscopy to determine volatility, ice nucleation activity, and water uptake on a single particle basis. Particle sources in the marine environment include regional sea spray, new particle formation, and long-range transport among others. This work demonstrates the impact of different marine aerosol particles collected at distinct layers of the atmosphere through chemical characterization as well as simulating particle properties during the processes of water uptake and ice nucleation.

2AC.1

Organic Aerosol from Chlorine-Initiated Oxidation of Hydrocarbons. LEA HILDEBRANDT RUIZ, Dongyu S. Wang, Surya Venkatesh Dhulipala, Sahil Bhandari, Catherine Masoud, Kanan Patel, *University of Texas at Austin*

Chlorine atoms (Cl) are much more reactive than hydroxyl (OH) and ozone (O_3) and can oxidize functional groups or whole molecules that are resistant to OH and O_3. Cl can also initiate radical propagation pathways which generate OH as secondary radical. Thus, Cl can rapidly initiate the oxidation cascade that results in the formation of organic aerosol (OA). Tropospheric chlorine chemistry has not received as much attention because its importance was believed to be limited to coastal areas. However, recent ambient measurements have detected high concentrations of reactive chlorine species in inland and mid-continental regions, suggesting that chlorine chemistry is also important in continental regions. In addition, due to its use as a disinfectant, chlorine chemistry can be important in the indoor environment.

Here we summarize results from laboratory experiments conducted in our group, which show efficient formation of OA from chlorine-initiated oxidation of different hydrocarbon precursors including isoprene, toluene, butyl carbitol and alkanes. Using measurements from a high resolution time of flight chemical ionization mass spectrometer (CIMS), we have tracked several generations of oxidation chemistry leading to the formation of organic particulate matter. We measured known and identified previously unknown reaction products of Cl-initiated oxidation, including highly oxidized molecules (HOMs). Using a filter inlet for gases and aerosols (FIGAERO) we analyze the molecular composition of organic aerosol and have found that Cl-initiated oxidation can form larger and lower-vapor pressure compounds than OH-initiated oxidation, which likely contributes to the larger aerosol mass yields often observed from Cl-initiated chemistry. OA formed from Cl-initiated reactions is often also more oxygenated than OA formed from OH-initiated chemistry.

The fast reaction rate of Cl with hydrocarbons enables complete consumption of all hydrocarbon precursors, including toluene, during an environmental chamber experiment. We evaluated the aging of toluene SOA by adding oxidant precursors after all toluene had been consumed. The addition of oxidants did not result in a significant change in the OA oxidation state, suggesting that the system may have reached an oxidative end-point in the particle phase. Organochlorides formed from all precursors investigated, even when the initial oxidation occurred via hydrogen-abstraction. Overall, our data suggest that chlorine chemistry can enhance atmospheric reactivity and increase the formation and transformation of organic aerosol. Cl-initiated formation of OA is currently not represented in air-quality models used to support the development of environmental policies; we argue that it should be.

2AC.2

Formation of Highly Oxidized Multifunctional Organic Compounds from Chlorine Atom Initiated Oxidation of α-pinene. Yonghong Wang, MATTHIEU RIVA, Xie Hongbin, Liine Heikkinen, Simon Schallhart, Otso Peräkyla, Chao Yan, Markku Kulmala, Mikael Ehn, *University of Helsinki*

Highly oxygenated molecules (HOMs) from the oxidation of monoterpenes in the atmosphere can irreversibly condense onto particles and contribute to secondary organic aerosol formation. Recently, the formation of nitryl chloride (ClNO2) from heterogeneous reactions, and subsequent photolysis, to produce chlorine atoms is suggested to be extensive not only in coast area, but also in urban region. However, the oxidation of monoterpenes such as α-pinene by chlorine radicals has received very little attention, and the ability of this reaction to form HOMs is completely unstudied. Here, chamber experiments were conducted with a-pinene and chlorine gas under low NO and high NO conditions, respectively. A NO3-based CI-APi-L-TOF was used to measure highly oxidized products. Clear distributions of monomers with 9-10 carbon atoms and dimers with 18-20 carbon atoms were observed under low NO conditions. With increased concentration of NO in the chamber, the formation of dimers was suppressed due to the competing reactions of peroxy radicals with NO. We calculated the HOM yields from chlorine-initiated oxidation of a-pinene under low NO conditions, while the yield at high NO could not be determined because of interference from ozone produced from the NOx, which subsequently reacted with a-pinene. Our study demonstrates that chlorine radical initiated oxidation of a-pinene will produce low volatility organic compounds, such as HOMs, which indicates that autoxidation processes in chlorine radical oxidation of a-pinene can be important. Further analysis will provide insights on the expected importance of the studied reactions in the atmosphere.

2AC.3

Probing the Role of Water in Criegee Chemistry Leading to High Molecular Weight Compounds on Aqueous Organic Surfaces. LIJIE LI, Michael Hoffmann, Agustin Colussi, *California Institute of Technology*

Ozonolysis of unsaturated organic gas emissions is a fundamental process in the formation and growth of tropospheric aerosols. O_3 adds to olefinic double bonds to produce chemically activated ozonides, which decompose into reactive carbonyl oxide Criegee (CIs) intermediates. CIs can react with H_2O, SO_2, carboxylic acids, aldehydes and alcohols, undergo unimolecular isomerization and dissociation, or bimolecular self-reaction. The competition among different reaction pathways determines the fate of organics and their potential for aerosol formation and growth. Understanding the role of water in these processes is essential, given its pervasiveness in the atmosphere both in the gas and aerosol phases. Recent reports have pointed out that the fate of gas-phase CIs in the troposphere is in fact dominated by their reactions with (H_2O)n_clusters. The ozonolysis of low-volatility, hydrophobic vapors, however, largely takes place on air-aerosol interfaces, given their fast reactions with O_3(g) and the low solubilities of both reactants in water. It is important to realize that in the steep water density gradient at air-aerosol interfaces, chemistry may proceed along different pathways and at faster rates than similar reactions in bulk gas and aerosol phases. In this work, we investigate the roles of water in the ozonolysis of oleic acid (OL) at the aerial interface of aqueous aerosols.

We focused on the formation of high molecular weight (HMW) compounds during the interfacial ozonolysis of OL. OL dissolved in acetonitrile/water mixtures (AN/W) was exposed to O_3(g) for < 50 µs under atmospherically relevant 1 atm of N_2, 298 K conditions. Online electrospray mass spectrometry (o-ESI- MS), which probes in situ the composition of the interfacial layers where ozonolysis takes place within 1 ms, was used to search for HMW (> C_{18}), α-acyloxyalkyl hydroperoxides from the addition of H_2O to CI, and other C_9 products. We explored the participation of water in these processes by performing experiments using D_2O and $H_2{}^{18}O$ instead of H_2O in the AN/W solvent. We found that HMW formation increases linearly both with O_3(g) exposure and OL concentration in the bulk solution, but decreases upon increasing the molar fraction of water. The main findings are that water functions as a solvent in the ionization of OL, and as a reactant that affects HMW formation.

2AC.4

There's No Place Like HOM: Modeling Peroxy Radical Chemistry to Understand HOM Yields. MEREDITH SCHERVISH, Wayne Chuang, Neil Donahue, *Carnegie Mellon University*

Knowledge of gas-phase oxidation chemistry is central to our understanding of aerosols. While gas-phase products of a wide range of volatilities are produced via oxidation of emitted precursors, low and extremely-low volatility gas-phase organic compounds are especially important because of their contribution to growth of particles as well as to the nucleation of new particles. Recent experimental work has shown the presence of highly oxidized molecules (HOMs), having vapor pressures in LVOC to ELVOC range, formed from the oxidation of alpha-pinene in both field and laboratory studies. These compounds are formed when peroxy radicals from the initial precursor oxidation "auto-oxidize" allowing them to rapidly undergo multi-generational oxidation chemistry. This process, involving a high energy barrier and thus being highly temperature-dependent, competes with radical termination reactions with NO_x, HO_2, and other RO_2 radicals. Under different conditions, this competition results in vastly different stable products. Under low NO_x and high temperature conditions, auto-oxidation dominates the fate of peroxy radicals leading to highly oxidized, low (and extremely low) volatility products including highly oxidized dimers. Under high NO_x and/or low temperature conditions, radical termination reactions dominate leading to products that are less oxidized and have higher volatilities. This competition is crucial in our understanding of the formation of ELVOC dimers as the dimer formation reaction may be dependent on the ability of RO_2 radicals to cluster together, requiring that they themselves have a low enough vapor pressure. This work seeks to underline the importance of the competition between auto-oxidation and radical termination under different conditions and explore HOM formation in chamber experiments through modeling.

2AC.5

Understanding the Fate of Highly Oxygenated Molecules in the Particle Phase Using an Extractive Electrospray Ionization Time-of-Flight Mass Spectrometer (EESI-TOF). VERONIKA POSPISILOVA, Felipe Lopez-Hilfiker, Claudia Mohr, Wei Huang, David Bell, Liine Heikkinen, Josef Dommen, Urs Baltensperger, Andre S.H. Prévôt, Jay G. Slowik, *Paul Scherrer Institute*

Atmospheric aerosols have significant impacts on human health and Earth´s climate. The highly oxygenated molecules (HOMs) yielded by the oxidation of biogenic and/or anthropogenic precursors contribute to the formation and growth of new particles in the atmosphere due to their low saturation vapor pressures. The molecular identification of these oxidized species in the gas phase is possible via chemical ionization mass spectrometry (CIMS) techniques. However, their identification and behavior in the particle phase remains an open question as currently no instrumentation allows online aerosol measurement on molecular level without thermal decomposition and/or ionization- induced fragmentation.

We present real-time measurements of individual organic aerosol species formed in alpha-pinene oxidation experiments in an atmospheric simulation chamber, as well as their direct observations in a boreal forest in southern Finland using a novel extractive electrospray ionization time-of-flight mass spectrometer (EESI-TOF) developed at PSI. We demonstrate that the EESI-TOF enables real time analysis of highly oxygenated molecules in the particle phase, without fragmentation, at atmospherically relevant mass loadings. We will present the separation of different generations of aerosol components and compare the results with measurements conducted by a FIGAERO-CIMS (Filter Inlet for Gases and AEROsols coupled to a CIMS), a well-established semi-continuous technique for aerosol composition measurement.

The analysis from these techniques makes it possible to investigate the evolution of these molecules in the particle phase and assess the degree of decomposition and/or accretion reactions occurring during the particle aging. Particle phase fragmentations reactions could be an important process that might reduce the overall efficiency at which low volatility gas phase organics contribute to the aerosol mass. It is also speculated that accretion reactions can lead to oligomerization in the particle phase, which could lead to a less volatile and, therefore, a more persistent form of secondary organic aerosol. Here, we will present evidence for particle-phase decomposition reactions.

2AC.6

The Role of Highly Oxygenated Molecules in Determining the Composition of Ambient Ions in the Boreal Forest.

FEDERICO BIANCHI, Olga Garmash, Xucheng He, Chao Yan, Siddharth Iyer, Matti Rissanen, Matthieu Riva, Nina Sarnela, Tuukka Petäjä, Douglas Worsnop, Markku Kulmala, Mikael Ehn, Heikki Junninen, Ida Rosendhal, Risto Taipale, Zhengning Xu, *University of Helsinki*

It has been recognized the ions can play a crucial role on atmospheric aerosol formation via the ion-induced nucleation mechanism. In order to investigate the negative ions in the boreal forest we have performed measurements to chemically characterise the composition of negatively charged clusters containing highly oxygenated molecules (HOMs). Additionally, we compared this information with the chemical composition of the neutral gas-phase molecules detected in the ambient atmosphere during the same period. The chemical composition of the ions was retrieved using an atmospheric pressure interface time-of-flight mass spectrometer (APi-TOF-MS) while the gas-phase neutral molecules (mainly sulfuric acid and HOMs) were characterised using the same mass spectrometer coupled to a nitrate-based chemical ionisation unit (CI-APi-TOF). Overall, we divided the identified HOMs in two classes: HOMs containing only carbon, hydrogen and oxygen and nitrogen-containing HOMs or organonitrates (ONs). During the day, among the ions, in addition to the well-known pure sulfuric acid clusters, we found a large number of HOMs clustered with nitrate (NO_3^-) or bisulfate (HSO_4^-), with the first one being more abundant. During the night, the distribution of ions, mainly composed of HOM clustered with NO_3^-, was very similar to the neutral compounds that are detected in the CI-APi-TOF as adducts with the artificially introduced primary ion (NO_3^-). For the first time, we identified several clusters containing up to 40 carbon atoms. These ions are formed by up to four oxidised-pinene units clustered with NO3-. While we know that dimers (16–20 carbon atoms) are probably formed by a covalent bond between two-pinene oxidised units, it is still unclear what bonding formed larger clusters. Finally, diurnal profiles of the negative ions were consistent with the neutral compounds revealing that ONs peak during the day while HOMs are more abundant at night-time. However, during the day, a large fraction of the negative charge is taken up by the pure sulfuric acid clusters causing differences between ambient ions and neutral compounds (i.e. less available charge for HOM and ON).

2AC.7

The Fate of Highly Oxygenated Organic Molecules in Wet Acidic Aerosols. LIINE HEIKKINEN, Matthieu Riva, Otso Peräkyla, Qiaozhi Zha, Simon Schallhart, Matti Rissanen, Tuukka Petäjä, Mikael Ehn, *University of Helsinki*

Organic aerosol (OA) makes up a large mass fraction of tropospheric fine particulate matter, worldwide. OA commonly originates from gas-to-particle transition processes and in this case can be referred to secondary organic aerosol (SOA). Biogenic volatile organic compounds (BVOCs) are an important source of SOA. Among the BVOCs, monoterpenes (MT) represent a major fraction of organic compounds produced over forested areas. In the boreal forest, α-pinene (AP) contributes significantly to the SOA formation through the generation of highly oxygenated molecules (HOMs). Indeed, such compounds are expected to have low vapor pressures and to significantly contribute to the formation of new particles in the atmosphere. In the presence of NO_x, the formation of multifunctional organic nitrates (ONs) has been reported as well as their subsequent presence in the particle phase. While the importance of HOMs and multifunctional ONs in SOA formation has been demonstrated, their fate within the particle phase has received much less attention and remain uncertain/unknown. It is worth noting that such compounds are expected to contain a wide variety of functional groups and thus are presumably highly reactive within the condensed phase.

In the present study, we investigated the fate of particulate HOMs both in the boreal forest in Southern Finland (SMEAR II station) and in a newly constructed atmospheric simulation chamber (COALA chamber). The laboratory experiments focused on the ozonolysis of AP under atmospherically relevant conditions. Seed aerosols with varying acidities and liquid water contents were used in order to replicate the conditions observed in the boreal forest. The particles sampled in both field and laboratory studies were chemically characterized utilizing different mass spectrometric techniques, such as a Filter Inlet for Gases and AEROsols coupled with an iodide adduct Chemical Ionization Mass Spectrometer (FIGAERO-CIMS) and a High Resolution Aerosol Mass Spectrometer (HR-AMS). Both instruments have an extended time-of-flight chamber enabling a high mass resolution and thus a more detailed understanding of the mass spectra. Our results from the field reveal that the HOMs, especially the dimers, undergo further particle phase reactions in the presence of sulfate aerosols, producing high molecular weight oligomeric products. These results were later confirmed by targeted laboratory experiments in the COALA chamber and stress the importance of acid-catalyzed reactions. Our study highlights that aerosol acidity leads to fast particle phase processing influencing the physicochemical properties of MT-derived SOA. Finally, the chamber studies reveal the decomposition of the particulate multifunctional ONs formed from the ozonolysis of AP in wet acidic aerosols, which could impact the atmospheric NO_x cycling.

2AC.8

Constraining the Abundance of Oligomers in Monoterpene Secondary Organic Aerosol. CHRISTOPHER KENSETH, Yuanlong Huang, Ran Zhao, Nathan Dalleska, Caleb Hethcox, Brian Stoltz, John Seinfeld, *California Institute of Technology*

High molecular weight oligomeric compounds have been identified as significant components of both ambient and laboratory-derived monoterpene secondary organic aerosol (SOA), and have been implicated as key players in new particle formation and growth, particle viscosity, and cloud condensation nuclei (CCN) activity. Electrospray ionization mass spectrometry (ESI-MS), typically coupled with liquid chromatographic (LC) separation, is among the most widely used analytical techniques for characterizing the identity and abundance of SOA molecular constituents. Due to a lack of authentic standards, oligomers in monoterpene SOA are typically quantified using commercially available terpenoic acids as surrogates (e.g., *cis*-pinonic acid and *cis*-pinic acid). However, due to fundamental differences in the ionizing behavior of monomers and oligomers, namely that oligomers produce ions with more delocalized charge, we have found through a combination of experimental and computational approaches that the sensitivity of ESI-MS toward oligomers is approximately two to ten times higher than that toward monomers, suggesting that the mass contribution of oligomers to monoterpene SOA has been significantly overestimated in past studies. In this work, we synthesize a series of monoterpene-derived oligomeric compounds and characterize their ESI efficiencies both empirically and theoretically. Using these oligomers as more representative surrogates, we constrain the abundance of oligomeric products in SOA derived from the O_3-initiated oxidation of α- and β-pinene, the most abundant monoterpenes in the atmosphere (total global emissions estimated at 85 Tg yr^{-1}). This critical analytical aspect of SOA formation experiments constitutes a potentially significant source of systematic bias in chamber-derived parameterizations of SOA production from monoterpene oxidation.

2AP.1

Observation of Nucleation Size Particles in the Amazon. FLORIAN DITAS, Christopher Pöhlker, Henrique Barbosa, Joel Brito, Samara Carbone, Xuguang Chi, Bruna A. Holanda, Isabella Hrabe de Angelis, Tobias Könemann, Jing Ming, Mira L. Pöhlker, Maria Prass, Daniel Moran-Zuloaga, Marta Sá, Jorge Saturno, Hang Su, Jian Wang, David Walter, Stefan Wolff, Alessandro Araujo, Paulo Artaxo, Ulrich Pöschl, Meinrat O. Andreae, *Max Planck Institute for Chemistry, Mainz, Germany*

New particle formation (NPF) and subsequent growth of nanometer particles is on a global scale responsible for a substantial fraction of the total particle budget and the number of cloud condensation nuclei (CCN). Under pristine conditions, the particle contribution by NPF can be of particular significance when the activation of CCN to cloud droplets is mostly limited by the amount of available aerosol particles.

One of the few continental places to study atmospheric aerosols under near-pristine conditions is the Amazon rainforest. Here, we will present observations from the *Amazon Tall Tower Observatory* (ATTO) site, which is located about 150 km northeast of the city of Manaus. The ATTO site is equipped to measure microphysical, chemical, hygroscopic and optical particle properties well-above (325 m), close to (60 m) and below (5 m) the canopy.

Particle number size distributions inside and above canopy suggest, at least, two different types of new particle formation events or sources. In contrast to the well-established continental banana-like events, a large fraction of the observed events at ATTO features a burst-like character without subsequent growth.

These events, which are typically shorter than 1-2 hours, occur more often during the dry season and sporadically in the presence of fog. The burst-like character and the sharp gradients of particle number concentration might indicate local particle sources.

In contrast, a more regional increase of nucleation size particles is frequently observed during the wet season and, in combination with vertical transport, often related to convective rainfall. In this study we investigate different event classes of nucleation size particles, their sources and significance vertically resolved inside, close to and well-above the Amazon rainforest canopy.

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2AP.2

Investigation of Dependencies of the Condensation Behaviour on Automotive Exhaust Soot in Condensation Nuclei Counters. MARTIN KUPPER, Martin Kraft, Alexander Bergmann, *CTR Carinthian Tech Research, Villach, 9524, Austria*

Introduction: Condensation nuclei counters (CNC) are proven metrology devices for particle number (PN) concentration measurements, used in scientific, industrial and environmental applications alike and legally mandated for automotive exhaust characterisation. The condensation of the working fluid on the (nano)particles is known to depend on both, the particles and the working fluid. As presented already at the AAAR annual meeting 2017, the inherent potential of optimising and usefully exploiting fluid - particle matching remains largely untapped. Instead, n-butanol is presently used almost invariably for an undesignated mix of different aerosol particles. Similarly, condensation models assume spherical structures, neglecting the real, often highly complex surface structures of aerosol nanoparticles.

Methods: A correction model of the deviation in the effective CNC cutoff caused by the difference of a fractally shaped condensation nucleus to an ideal sphere was developed. This theory-based approach was backed by analysis of published counting efficiency curves using different nuclei and validated against this data. In a parallel effort, key factors describing particle species – working fluid interaction and resultant counting efficiency – have been compiled and are presently being experimentally examined using a dedicated research CNC with different working fluids and particle species and structures. To examine the dedicated influence of morphology on the nucleation process a study using small angle X-ray scattering (SAXS) on defined particles in a well-known CNC is in progress.

Results: Comparing the developed model with literature data indicates a strong dependency of nucleation efficiency on the respective material properties and furthermore a significant impact of the particle morphology. Both effects are hence significant for a correct determination of PN and a targeted further development of CNC-based aerosol analysers. Yet, the contributions of morphology and material matching to particle activation overlap and cannot be clearly and unambiguously separated experimentally. A test series was designed to settle this point by systematic examination of the nucleation on particles with different morphology but same material. By comparisons of the experimental results with the model, the correction of CNCs is further sharpened for measuring PN in automotive exhaust.

2AP.3

Quantifying Initial Nanoparticle Growth of Organic and Inorganic Systems with the CLOUD Experiment. DOMINIK STOLZENBURG, Lukas Fischer, Martin Heinritzi, Mario Simon, Katrianne Lehtipalo, Chao Yan, Lubna Dada, Paul M. Winkler, *University of Vienna*

New particle formation and subsequent nanoparticle growth has been identified as the main contributor to the global budget of cloud condensation nuclei (CCN), significantly impacting the Earth's radiative balance (Gordon et al. (2017), J. Geophys. Res.-Atmos., 122). In order to reach CCN sizes, high initial particle growth rates are crucial for the survival of freshly formed nanoparticles, at sizes below 10nm, as they rapidly coagulate with pre-existing aerosol. Characteristics of particle growth depend largely on the abundance of different condensable vapours and parameters such as temperature and relative humidity. Detailed studies exploring this wide parameter space are missing so far.

Here we present results from three measurement campaigns at the CERN CLOUD experiment (Duplissy et al. (2016) J. Geophys. Res. Atmos., 121, and references therein), exploring a wide range of parameters under precisely controlled conditions. Accurate quantification of sub-10 nm growth rates were achieved by using a DMA-train (Stolzenburg et al. (2017), Atmos. Meas. Tech., 10, 1639-1651) in combination with high-resolution mass spectrometry (Jokinen et al. (2012), Atmos. Chem. Phys., 12, 4117-4125; Breitenlechner et al. (2017), Anal. Chem., 89, 5824-5831).

Particle growth in several organic, inorganic and combined systems, including sulphuric acid, ammonia and highly oxidized molecules from alpha-pinene ozonolysis was measured in the temperature range between -50 and +25 °C. Moreover, experiments were performed for systems similar to those found in the atmosphere, by adding NOx and isoprene.

We find that the chemical system directly impacts the size-dependence of the growth rates and that especially the addition of NOx and isoprene influence the contribution of organics due to different resulting oxidation products. In this respect, also temperature plays a decisive role as volatility is the dominant parameter for the condensation of organic molecules. The resulting parametrization of growth rates with respect to condensable vapour concentrations will certainly help to improve the treatment of nanoparticle growth in global models. The insights gained into particle growth mechanisms by this set of experiments can possibly explain the occurrence of nanoparticle growth up to CCN sizes in various regions all over the globe.

2AP.4

Laboratory Study on the Impact of Organic Vapours on Water Uptake of Aerosols. DAWEI HU, David Topping, Gordon McFiggans, *University of Manchester*

Clouds have a profound influence on weather and climate. According to the Intergovernmental Panel on Climate Change (IPCC), the impacts of aerosols on clouds are one of the largest uncertainties in estimates of the global radiative forcing. The formation of cloud droplets by the condensation of water vapours on particles can be predicted by traditional Köhler theory, but this treatment is limited to involatile compounds with water vapour only and does not account for the influence of other inorganic or organic vapours. Previous modelling studies reported that co-condensation of inorganic or organic vapours on growing droplets could significantly enhance both cloud condensation nucleus (CCN) and cloud droplet number concentration, thereby influencing cloud albedo and climate. However, until now, there has been no direct observational evidence of this process.

Here, we use a modified Hygroscopic Tandem Differential Mobility Analyser (H-TDMA) system to investigate the growth of inorganic salt particles exposed to both water and organic vapours in the laboratory. The result shows that organic vapour plays an important role in water uptake process of aerosols consistent with our previous predictions. To our knowledge, this study reports the first direct measurement to quantify the influence of organic vapour on the water uptake of aerosols.

2AP.5

How Increased Ionization Can Boost Aerosol Growth to Cloud Condensation Nuclei. MARTIN BøDKER ENGHOFF, Henrik Svensmark, Nir Joseph Shaviv, Jacob Svensmark, *Technical University of Denmark*

In this study (Svensmark et al, 2017) the effect of ionization on the growth of aerosols into cloud condensation nuclei is investigated theoretically and experimentally. We show that the mass-flux of small ions can constitute an important addition to the growth caused by condensation of neutral molecules.

Under atmospheric conditions the growth from ions can constitute several percent of the neutral growth. We performed experimental studies which quantify the effect of ions on the growth of aerosols between nucleation and sizes up to 20 nm and find good agreement with theory. Ion-induced condensation could be of importance not just in Earth's present day atmosphere for the growth of aerosols into cloud condensation nuclei under pristine marine conditions, but also under elevated atmospheric ionization caused by increased supernova activity.

We propose an addition to the condensation equation based on the additional mass-flux of ions to aerosols. The expression depends on the ratio of the number concentration of ions to the number concentration of neutrals, the ratio of the interaction coefficient between ions and neutral aerosols to the interaction coefficient between neutral molecules and aerosols, the ratio of the ion mass to the neutral mass, and finally the ratio of the amount of neutral aerosols to the total amount of aerosols. While the second and fourth terms are (nearly) constant under most conditions the ion/neutral number concentrations and mass vary depending on atmospheric conditions. In a pristine environment at high ionization levels the effect can account for almost 20% of the growth rate of small aerosols and a significant enhancement up to 20-30 nm.

The theory was tested experimentally in 7 m^3 atmospheric reaction chamber, measuring the aerosol size distribution and (for some of the experiments) the sulphuric acid concentration. A total of 3100 hours of data with varying gas and ion concentrations were analyzed. For each set of experimental conditions a number of experiments where ionizing gamma sources were opened and closed with typically 2 hour intervals were performed. We then superposed the individual experiments onto each other to reveal the growth profile with and without increased ionization. Analyzing these superposed growth profiles allowed us to compare growth rates with and without ionization to the theory and we found a good agreement between the two.

The mechanism is favoured by high ionization, low gas concentrations, and low aerosol concentrations. This points to pristine settings, such as over oceans away from continental and polluted areas. Potentially the mechanism can contribute significantly to the production of cloud condensation nuclei, but to fully assess the impact the mechanism should be included in global climate simulations.

Svensmark, H., Enghoff, M. B., Shaviv, N. J., and Svensmark, J. (2017). Nat. Commun., 8:2199.

2AP.6

Ageing of Sea Spray Aerosols: Effects on Hygroscopicity and Cloud Droplet Activation. BERNADETTE ROSATI, Sigurd Christiansen, Robert Lange, Andreas Massling, Merete Bilde, *Aarhus University*

Sea spray aerosols (SSA) are continuously emitted into the Earth's atmosphere and play a significant role in the planetary energy budget, by interacting directly with solar radiation and by affecting the formation and lifetime of clouds. This has a major effect on climate since 70% of the planet is covered by the ocean, which thereby is the largest single source of aerosol mass in the atmosphere (e.g. de Leeuw et al. 2011). The atmospheric lifetime of SSA varies from seconds to weeks. During this time, SSA is exposed to oxidants, condensable vapors, light and changing conditions of relative humidity and temperature, which induce so-called ageing effects. Hence, the properties of SSA may be significantly altered, which leads to changes in their role for climate.

The hygroscopic behavior of SSA, at sub- saturated conditions of relative humidities (RH), influences the type and magnitude of the aerosol-radiation interactions because the optical properties of the aerosol particles change due to water uptake. The hygroscopicity may also affect the particles' efficiency to act as cloud condensation nuclei (CCN) at supersaturated conditions. Commonly, the hygroscopicity and CCN-activity of SSA is assumed to be comparable to that of sodium chloride (NaCl; Lewis and Schwartz, 2004), which is the major component of SSA particles overall (Lewis and Schwartz, 2004). Previous laboratory studies have investigated reactions of aqueous NaCl with ozone and the presence of UV-light, hereby mimicking ageing conditions occurring in the marine boundary layer (Knipping et al., 2000, Laskin et al., 2003). These experiments demonstrated changes in the chemical and physical properties of the particles and hence the authors hypothesize a possible effect on the hygroscopic and cloud activation potential.

In this study, we examine the hygroscopic and cloud forming potential of SSA after atmospheric ageing processes. To simulate different atmospheric conditions, we use the constrained conditions of the Aarhus University Research on Aerosol (AURA) smog chamber (Kristensen et al., 2017), which provides a temperature regulation between 257 and 299 K. In our experiments, the chemical composition of SSA is first simplified by using pure NaCl particles generated with a TSI atomizer. In a second step, another generation technique, i.e. a sea spray chamber, and more complex mixtures of inorganic salts are used. Hygroscopicity is measured with a humidified tandem differential mobility analyzer (Brechtel) while a cloud condensation nucleus counter (DMT) is used to investigate the cloud droplet activation of the fresh and aged particles. Additionally, the particle number size distribution is monitored with a scanning mobility particle sizer (SMPS; TSI) and an optical particle sizer (OPS; TSI). We will present first results of ageing experiments, where NaCl undergoes oxidation due to gases and UV-radiation as present in the atmosphere. We will show that only deliquesced NaCl particles lead to chemical reactions influencing the hygroscopic and CCN-activity and that the results strongly depend on the pre-treatment of the aerosol particles.

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2AP.7

A Unifying Identity for the Work of Cluster Formation in Heterogeneous and Homogeneous Nucleation Theory.

ROBERT MCGRAW, Paul M. Winkler, Paul E. Wagner, *Brookhaven National Laboratory*

Nucleation in the atmosphere is responsible for the formation of new particles that can subsequently grow to exert a significant impact on global climate directly through the scattering and absorption of solar radiation and indirectly by serving as sites for cloud droplet condensation. There is evidence that both homogeneous nucleation and heterogeneous nucleation pathways contribute to this process. Indeed, the interesting two-stage model of Kulmala and co-workers: heterogeneous nucleation of (most likely) oxidized organic vapors on stabilized 1-2 nm neutral cluster condensation sites formed from the gas phase, effectively eliminates distinction between heterogeneous and homogeneous nucleation mechanisms as the condensation sites approach molecular size. A unifying identity is derived in the present study relating the surface and volume components of the reversible work of cluster formation. Shown to generalize two early thermodynamic relationships of Gibbs, the new result is demonstrated here for Fletcher's model of heterogeneous nucleation on flat and curved substrates and in the homogeneous nucleation limit, for clusters of non-critical as well as critical size, and for application to non-classical (molecular-based) theories. The new identity can serve as a check on the consistency of complicated theoretical expressions and numerical calculations and help guide interpretation of measurements.

2AP.8

Controlling and Explaining the Formation of Bimodal Aerosol Distributions in Laboratory Studies. Phoebe Belser, Hemanta Timsina, Dabrina Dutcher, TIM RAYMOND, *Bucknell University*

Because of the abundance of dicarboxylic acids in the atmosphere, they are commonly studied in the aerosol field, specifically investigating their hygroscopic and cloud condensation nuclei activity properties along with their behavior in inorganic mixtures. Glutaric acid, being a water soluble dicarboxylic acid is commonly used to model water activity in dicarboxylic acid aerosols. Studying trends associated with glutaric acid aerosols in the atmosphere, such as CCN activity and water uptake behavior is common. Glutaric acids behavior in the presence of inorganic particles, such as coating inorganic aerosols and forming co-crystals, is also frequently studied. However, in several circumstances there is some variability within the data associated with glutaric acid, specifically DRH and hygroscopic data, which is hypothesized to be caused by its polymorphism.

Glutaric acid exhibits dimorphism, meaning the molecule can form into two different types of crystal structures, an alpha and a beta polymorph, which can manefest themselves as a bimodal aerosol size distribution when analyzed by SMPS or other mobility sizing methods. Glutaric acid naturally forms in the beta polymorph, which is more stable. The alpha polymorph is the metastable phase, meaning it is less stable. In this work we investigated the formation of the alpha glutaric acid polymorph in aerosols generated from an aqueous glutaric acid solution. In no published research has the formation of both polymorphs from an aqueous solution been documented. Identifying the presence of polymorphism in glutaric acid aerosols will ideally explain the variability present in studies associated with glutaric acid aerosols. Understanding and defining under which conditions the alpha polymorph is present will allow others to avoid it when investigating glutaric acid as a dicarboxylic acid.

Additionally, bimodal distributions have been observed with select mixtures of organic and inorganic substances, however the mechanism creating biomodality appears to be different than polymorphism. These results will be presented and explained.

2CA.1

Understanding the Physical and Optical Properties of Black Carbon Aerosols at Delhi and Kanpur in Indo-Gangetic Plain. NAVANEETH M. THAMBAN, S.N. Tripathi, Shamjad P.M., *IIT Kanpur*

The mass concentration, size distribution, and absorption properties of black carbon (BC) aerosols were measured at two different sites in the Indo-Gangetic Plain (IGP) for improving the radiative forcing calculations. A Single Particle Soot Photometer (SP2) and Photo Acoustic Soot Spectrometer (PASS-1) were operated at Kanpur and Delhi for the year of 2015 and 2018 respectively during the winter season. The mean mass absorption cross-section values (MAC_{781}) for Delhi was slightly higher than that of Kanpur (11.04 m^2/g, 10.1 m^2/g respectively) during the sampling period. The relative lower mode BC number size distribution at Delhi suggested the presence of nearby BC sources in Delhi than Kanpur. In addition, the higher variability in the BC number to mass ratio indicates the heterogeneity in the BC sources in Delhi than Kanpur.

2CA.2

Influences of Primary Emission and Secondary Coating Formation on the Mixing State of Black Carbon-containing Particles.

ALEX LEE, Chia-Li Chen, Jun Liu, Derek Price, Raghu Betha, Lynn Russell, Xiaolu Zhang, Christopher Cappa, *National University of Singapore*

Black carbon (BC) emitted from incomplete combustion can result in significant impacts on air quality and climate. Understanding the mixing state of ambient BC and the chemical characteristics of its associated coatings is particularly important to evaluate BC fate and environmental impacts. In this study, we investigate formation of coating on BC particles and aerosol mixing state near traffic emissions under hot and dry conditions in Fontana, California using an Aerodyne soot-particle aerosol mass spectrometer (SP-AMS). The SP-AMS was operated in a configuration that can exclusively detect refractory BC (rBC) particles and their non-refractory coating materials, including organic, nitrate, sulfate, ammonium and chloride.

Substantial formation of secondary organic aerosol (SOA) coatings on rBC particles was observed due to active photochemistry in the afternoon, whereas primary organic aerosol (POA) components were strongly associated with rBC from fresh vehicular emissions in the morning rush hours. Nitrate peaks were observed in the late morning due to formation of nitric acid via OH radical oxidation of NO2 in traffic emissions. Using the −log(NOx ⁄ NOy) ratio as a proxy for photochemical age of air masses, most of the observed SOA coatings were freshly formed, providing an opportunity to examine SOA coating formation on rBCs near vehicular emissions. Comparison of our results to a co-located standard high-resolution time-of-flight aerosol mass spectrometer (HR-ToF-AMS) measurement suggests that approximately 7–20 wt % of secondary organic and inorganic species were estimated to be internally mixed with rBC on average, implying that rBC is unlikely the major condensation sink of secondary species.

Event Trigger mode of SP-AMS was used to measure chemical composition of individual rBC-containing particle. Preliminary results of cluster analysis of single-particle measurements indicate the presence of various types of primary and secondary coatings based on their mass spectral characteristics. The mixing state index, χ, was calculated for quantifying the degree of mixing of rBC and coating materials (i.e., χ = 0 and 1 means that all particles are fully externally and internally mixed, respectively). The mixing state index varied between 0.2 and 0.6 with the average of 0.38 (± 0.06) in this study, and was not sensitive to the photochemical age of air masses. Nevertheless, the average particle species diversity (D_α) and the bulk population species diversity (D_γ), which represent the average effective number of species in each particle and the effective number of species in the population, respectively, slightly increased with primary traffic emissions and/or nitrate formation but gradually decreased with SOA formation during the afternoon. These observations indicate that substantial SOA formation observed in the afternoon led to more homogeneous particle compositions.

2CA.3

Black Carbon Aerosol in a Clean Marine Environment. WALT WILLIAMS, Armin Sorooshian, Haflidi Jonsson, Richard Flagan, John Seinfeld, Andrew Metcalf, *Clemson University*

Black carbon (BC) aerosol was measured with a Single Particle Soot Photometer (SP2) in a relatively clean, marine environment in the Eastern Pacific, just off the central coast of California. In this region, direct emission of BC aerosol comes mostly from the shipping industry, with occasional inputs from biomass burning in California (although most emissions over land are carried eastward across the continental United States). Some BC aerosol in the region is from long-range transport from Asia. Regardless of BC source, the mixing state of individual BC aerosol particles can have a large effect on its climate-forcing potential and lifetime in the atmosphere. Recent results from other studies in remote marine environments show that some regions are characterized by uncoated BC, while other regions have nearly all BC aerosol mixed with water-soluble materials.

In this talk, measurements of BC mass, size distribution, concentration, and mixing state will be presented for a clean marine environment from 2 sampling campaigns: from summer of 2011 and summer of 2018. BC aerosol measurements will be compared to other measurements of total aerosol size, concentration, and chemical composition. One goal of this study is to use the BC mixing state information from the SP2 measurements to identify new emission sources of BC aerosol versus BC from long-range transport. To accomplish this goal, measurements from near-ship will be compared to those above the boundary layer to identify plume profiles from different aerosol sources. Another goal of this study to examine BC characteristics in droplet residual particles in relation to other inorganic and organic constituents. To accomplish this goal, some sampling periods were behind a counterflow virtual impactor. Finally, characteristics of long-term trends in BC aerosol in this region will be inferred from a comparison of these sampling campaigns 7 years apart.

2CA.4

Quantifying Black Carbon Light Absorption Enhancement with a Novel Statistical Approach. Cheng Wu, Dui Wu, JIAN ZHEN YU, *Jinan University*

Black carbon (BC) particles in the atmosphere can absorb more light when coated by non-absorbing or weakly absorbing materials during atmospheric aging, due to the lensing effect. In this study, the light absorption enhancement factor, E_{abs}, was quantified using a 1-year measurement of mass absorption efficiency (MAE) in the Pearl River Delta region (PRD). A new approach for calculating primary MAE (MAE_p), the key for E_{abs} estimation, is demonstrated using the minimum R squared (MRS) method, exploring the inherent source independency between BC and its coating materials. A unique feature of E_{abs} estimation with the MRS approach is its insensitivity to systematic biases in elemental carbon (EC) and σ_{abs} measurements. The annual average E_{abs550} is found to be 1:50±0:48 (1 SD) in the PRD region, exhibiting a clear seasonal pattern with higher values in summer and lower in winter. Elevated E_{abs} in the summertime is likely associated with aged air masses, predominantly of marine origin, along with long-range transport of biomass-burning-influenced air masses from Southeast Asia. Core– shell Mie simulations along with measured E_{abs} and absorption Ångström exponent (AAE) constraints suggest that in the PRD, the coating materials are unlikely to be dominated by brown carbon and the coating thickness is higher in the rainy season than in the dry season.

2CA.5

Impact of Diesel Container Truck Emissions on Carbonaceous Aerosols in a Unique Roadside Environment in Hong Kong.

YEE KA WONG, Jian Zhen Yu, *Hong Kong University of Science and Technology*

Street-level air pollution is a major concern in Hong Kong, and over the years the Government has implemented a series of measures to reduce the vehicular emissions, particularly those from diesel commercial vehicles. This work demonstrates multiple approaches in estimating vehicular contribution to $PM_{2.5}$, which potentially serves as the basis for evaluating the ongoing vehicle emissions control policies. A Sunset Laboratory semi-continuous OC-EC field analyzer was deployed to measure the hourly concentrations of $PM_{2.5}$ organic carbon (OC) and elemental carbon (EC) at Lok Ma Chau Control Point (LMC), an ad hoc roadside site in Hong Kong, in 9 selected months from 2015 to 2017. The site is located in an open area near the boundary between Hong Kong and Mainland China, and is characterized as being heavily impacted by the exhaust from diesel container trucks passing by en route to Mainland China. The monthly average (± standard deviation) OC ranged from 2.89 ± 1.94 to 7.10 ± 3.41 μgC/m^3, with a higher contribution in winter mainly due to regional transport. EC ranged between 1.98 ± 1.24 and 4.01 ± 1.70 μgC/m^3, and is found strongly associated with diesel goods vehicle number when diurnal and weekday-holiday patterns were investigated. A very low traffic volume period during Chinese New Year (CNY) holiday was also captured, during which the rush hour EC plummeted to 1.13 ± 0.38 μgC/m^3, compared to 3.93 ± 1.43 μgC/m^3 outside the CNY period. The multiple pieces of evidence further corroborate EC as the effective tracer for diesel vehicular exhaust. In view of this and the roadside characteristics of the sampling site, $PM_{2.5}$ from vehicular exhaust (PM_{veh}), equivalent to the sum of EC and vehicle-related organic matter, was estimated through EC-tracer method. The OC-to-EC ratio of vehicular exhaust was determined to be 0.53 based on the optimal Deming regression using the lowest 5% data by OC/EC ratio from summer. The distribution of the selected data aligned well with the diurnal traffic volume pattern. On a monthly basis, the PM_{veh} were between 3.45 ± 2.17 and 6.99 ± 2.96 μg/m^3. PM_{veh} was also estimated independently by positive matrix factorization (PMF) considering major species and organic tracers (including hopanes) derived from 24-hr filter-based measurements at the same roadside site and one nearby general site. The results are tightly consistent with each other. For the overlapping samples the ratio in PM_{veh} between the two approaches is 1.04 ± 0.45, while that for vehicular OC is 0.89 ± 0.39 ($n = 22$), adding credence to the two approaches in providing estimation of PM_{veh}. Based on the PMF results, the vehicular exhaust was responsible for 14.6% of $PM_{2.5}$ and 19.3% of OC at LMC site.

2CA.6

Development of Size-resolved Black Carbon Particle Number Emission Inventory for Global Civil Aviation. XIAOLE ZHANG, Xi Chen, Jing Wang, *ETH Zuerich*

The air traffic is growing rapidly. The black carbon (BC) in the aviation exhaust may impact climate, environment and public health. The particle number and size distribution are relevant metrics for toxicological analysis and aerosol-cloud interactions.

In this study, a size-resolved BC particle number emission inventory is developed for the global civil aviation based on the recent measurements. The development follows the European Environment Agency (EEA) air pollutant emission inventory guidebook by utilizing the global scheduled flight dataset in 2005. The BC mass emission indices for nearly 300 types of aircrafts under various flight conditions are also provided by EEA. The mass-number conversion is conducted using fractal aggregate theory and the particle mass parameters obtained from experiments. The geometric mean diameters (GMD) and geometric standard deviations (GSD) of the particles are estimated with a new correlation based on the combustor inlet temperature (T_3) and BC mass emission index (EI_m) of the aircraft engines. Other flight parameters (e.g. speed, altitude, duration) are defined based on the statistics of thousands of Automatic Dependent Surveillance-Broadcast (ADS-B) and Flight Data Recorder (black box) records.

The number of civil aviation emitted BC particles is estimated to be 1.09×10^{26} per year (with 95% prediction interval of $6.8\sim15.0\times10^{25}$ per year) and the mass emission 9.5 Gg per year. The LTO cycles below 3000 ft (taxi, take-off, climb-out, and approach) and CCD (climb, cruise, and descent) above 3000 ft respectively account for 10.2% and 89.8% of the total particle number. The global mean BC GMD is the largest in take-off, then climb out, climb and cruise. The approach, taxi, and descent phases have the lowest GMDs. The global mean GSDs of different phases are all comparable, within a narrow interval between 1.80 and 1.85. The results indicate that the civil aviation has a much higher contribution to the total anthropogenic particle number emission than that to the mass emission.

Significant spatial heterogeneity has been observed. The number and mass emissions in Asian, Europe, America and other markets are related to the air traffic volume but subjected to modulation by the airplane type. The number emission index varies from about 5.5×10^{14} per kg-fuel in Northern America to 1.2×10^{15} per kg-fuel in C.W. OF IND. STATES due to the significant spatial variations in GMDs (about 29 nm in Northern America and 38 nm in C.W. OF IND. STATES.), which is mainly caused by the different dominant airplane types.

The developed emission inventory can be used as input data for air quality/climate models. The uncertainties in the inventory need further investigation.

2CA.7

Physico-chemical Characterization of Small-scale Gas Flaring. Alberto Baldelli, Ramin Dastanpour, Una Trivanovic, Melina Jefferson, Jason S. Olfert, Alireza Moallemi, Kevin Thomson, Matthew Johnson, Olga Popovicheva, STEVEN ROGAK, *University of British Columbia*

The properties of particulate emissions affect their impact on the environment and the human health. Flaring operations in the oil and gas industries can be major sources of soot, but are presently not well characterized. Carleton University has a laboratory flame that approaches the scale of a small industrial flare. This facility was used to study emissions relevant to flaring in Canadian oil and gas production. Three fuel compositions (mixtures of methane, ethane, propane, butane, N2, and CO2), a range of exit velocities (0.5 to 1.5 m/s), and burner diameters of 38, 51, and 76 mm were studied.

A broad suite of optical, physical, and chemical characterization techniques was used to allow a comprehensive characterization of the gas flare particulate emissions. Individual particles were analyzed using High Resolution Transmission Electron Microscopy (HRTEM), Raman Spectroscopy, and Scanning Electron Microscopy coupled by Energy Dispersive X-ray (SEM-EDX) spectroscopy. Furthermore, a Fourier transform infrared (FTIR) was used on bulk samples of soot for a deeper analysis of its chemical structure. The major type is soot distinguished by agglomerates of ultrafine primary particles of 30 ± 10 nm diameter containing from a few up to hundreds of spheres. HRTEM images are characterized by the length, tortuosity and separation of individual graphene fringes in soot. Analysis of Raman spectroscopy is sensitive to the degree of graphitization and crystal sizes in disordered carbon. We found here that Raman spectra were very similar for soot from all fuels considered. From EDX we found that as expected, every particle was composed mainly of C and O. Cluster analyses of composition data proposes the separation of into characteristic groups representative of various gaseous fuel mixtures and operation conditions. Group “Elemental Carbon” accounts for 86 to 97% of particles while Group “Oxidized Soot”, which are for the 70% made of oxygen, appeared with abundance of a few percent.

Characterization of bulk composition by thermo-optical transmission (TOT) method using a semi-continuous OC/EC analyzer with organic vapour trap, showed the particulate to have a very high elemental to total carbon (EC/TC) ratio across all flare test points. For the organic fraction, FTIR spectra shows the major classes of organic compounds determined by aliphatic C-C-H, aromatic C=C, and carbonyl C=O functionalities.

2CA.8

Inter-Comparison of Techniques for the Measurement of Black Carbon from Biomass Burning: Influence of Optical and Chemical Properties. HANYANG LI, Kara D. Lamb, Joshua P. Schwarz, Vanessa Selimovic, Robert J. Yokelson, Gavin McMeeking, Andrew May, *The Ohio State University*

Biomass burning is a major contributor to global black carbon (BC) emissions. However, the exact magnitude of BC emissions from biomass burning is difficult to examine due in part to highly variable combustion conditions and irregular spatiotemporal repeatability (e.g., wildfire emissions do not follow a regular weekly pattern throughout the year). An additional complication is that there are many approaches that can be used to measure BC emissions. Predominant methods in use today represent one of three distinct operationally-defined quantities: “equivalent” BC (eBC), “refractory” BC (rBC), and elemental carbon (EC). Given that EC might be used to represent eBC or rBC, and vice versa, it is essential to understand the relationship among BC measurements, and develop robust BC emission factors for biomass burning.

To systematically assess BC measurement techniques and investigate the uncertainties of BC emissions from biomass burning, we participated in the Fire Sciences Laboratory studies in Missoula, MT during Autumn 2016 as part of the Fire Influence on Regional and Global Environments Experiment (FIREX). Eight real-time instruments were deployed sharing the same smoke inlet, including two in situ methods for eBC, five filter-based methods for eBC, and one method for rBC; furthermore, quartz filters were collected for off-line thermal-optical analysis of EC. There have been similar prior efforts, but none that focused on biomass burning smoke have been this comprehensive (and none have compared EC and rBC). This presentation extends our previous work to compare EC with light-absorption measurements of BC. Quartz and quartz-behind-Teflon® filter samples containing EC and OC are analyzed using Sunset Laboratory OCEC analyzer by IMPROVE-A temperature protocol. Such filter data is also used to calculate organic aerosol concentration (C_{OA}), bare-quartz organic mass (OM) and particle-phase organic mass fraction (X_P), and thus we can evaluate the effect of OA gas-particle partitioning on emission factors of BC.

In our presentation, the association between BC uncertainties and intercorrelated optical and chemical properties of biomass burning (e.g. single scattering albedo, angstrom absorption exponent, absorption enhancement, C_{OA}, and OC/EC ratio) will be illustrated using both statistical methods and an alternative graphical/parametric approach. Our results indicate that both fixed and proportional biases are present among instruments. Fixed biases exist when comparing three general BC techniques (as well as various instruments using the same measurement technique). Measurements of BC may be also biased either high or low depending on aerosol properties and OA gas-particle partitioning, which is classified as proportional biases. This work will encourage accurate quantification of BC emissions from biomass burning and improve the predictions of climate and chemical-transport models.

2CM.1

An Integrated Modeling and Optimized Operating Method for Electrostatic Precipitation Process of Particulate Matters. YISHAN GUO, Yueqi Huang, Chenghang Zheng, Weiguo Weng, Yi Wang, Xiang Gao, *Zhejiang University, China*

Electrostatic precipitators (ESPs), widely utilized as the main particulate matter(PM) removal facility in flue gas treatment system of coal fired power plants, are high power consuming facilities consisting dozens of high voltage power supplies. Existing operating methods, lacking the comprehensive understanding of PM removal process and its relationship with energy consumption, could not fully cultivate the energy saving potential, and the feedback methods for operation voltage was unable to maintain a reliable outlet concentration. In this article, an integrated model, considering both precipitation mechanism of particulate matters together with the energy consumption, was put forward to monitor the operation of ESPs under varying operation parameters. The charging, migration and removal behavior of particulate matters under different energy injection level in wire-duct ESPs was comprehensively studied and the model to predict the outlet concentration was corrected through real operation data. At the same time, the emission distortion introduced by load shifting, flow distribution, ramping, etc., was analyzed. Based on the integrated model, coordinated operation set points for multiple cascaded and parallel discharging fields were achieved utilizing optimized operating method. In order to ensure the compliance rate of outlet concentration, a unique emission preferential method, which modifies the corrections of operation set points according to the optimized value together with the real time emission, was created and the optimized set points were compared with the real time operating point to get the correction gain and modify the operation set point to meet the emission goal. The method was adopted at an industrial ESP and a 100% of hourly compliance rate with more than 30% energy consumption reduction was achieved.

2CM.2

Pollutant Emissions from Steelworks Equipped with Various Flue Gas Desulfurization Systems. QING LI, Di Wu, Xiang Ding, Xianmang Xu, JianMin Chen, *Fudan University*

China has been the largest steel producer since 1997, and has accounted for about a half of the total world steel production since 2013. Pollutant emissions from sintering machines of steelworks is one of the largest contributor to China’s PM2.5 pollution. Compared to the great efforts made to limit emissions from coal-fired power plants, the percentage of air pollution control devices installed in steelworks is much lower, e.g. flue gas desulphurization systems (FGD) are used in less than 40% of the steelworks. This is due to less public concern and very complex flue gas composition, which has challenged the current FGD technologies.

This study compares removal efficiencies of various pollutants by using active coke, ammonia, and limestone FGD systems based on field measurements. The three FGD systems were installed to clean flue gases for three typical sintering machines, all of which used the same combustion technologies and fuels. The capacity of sintering machine equipped with the dry FGD system (active coke) is 600 m2, while that of the other two wet FGD system (ammonia and limestone) are both 360 m2. Wet electrostatic precipitators were installed for both wet FGD systems. It was found that the efficiency to remove SO2 was sufficient for all the three FGD technologies (>98%). However, compared to the other systems the ammonia FGD is less efficient in removing SO3, which may contribute to primary particulate matter in the flue plumes. Moreover high concentrations of ammonia (2021 mg/ m3) were observed in the flue plume after the ammonia FGD. These high ammonia concentrations are probably caused by carryover from the ammonia FGD system, and should be addressed in the future. Furthermore, compared to the other systems a higher concentration of soluble ions after ammonia FGD was detected owing to the lower removal efficiency of SO3 and slip of ammonia from the FGD system. Comparing dust concentrations at FGD inlets and outlets, the dust concentration in ammonia and limestone FGD outlets were decreased by 61% and 50%, respectively, while that at the active coke FGD outlet was increased by 5%.

To conclude, although all three FGD technologies are effective in removing SO2, the high rate of ammonia slip from ammonia FGD system should be considered, as well as its low efficiency in removing SO2. According to our results we recommend the limestone FGD technology for cleaning flue gases from sintering machines in steelworks.

2CM.3

Sampling Efficiency of PM10 Inlets with Different Impaction Substrates. THI-CUC LE, Krishna Kumar Shukla, Jung-Che Sung, Jia Feng, Ziyi Li, Chuen-Jinn Tsai, *National Chiao Tung University*

The EPA louvered PM10 inlet (16.7 L/min) is commonly used in PM10 FRM samplers or FEM monitors. The particle collection efficiency of the PM10 inlet is influenced by the wind speed, particle bounce and particle overloading. To study the effect of wind speeds, the sampling efficiency of PM10 inlet was calculated as the product of the particle collection efficiency of the PM10 impactor determined in our laboratory with the sampling effectiveness of TSP inlet at different wind speeds (Vanderpool et al., 2018). The test results of the particle collection efficiency of the impactor showed the cut-size of 10.29 ± 0.07 µm and sharpness of 1.37 ± 0.03, which are very close to those determined from the sampling efficiency of the PM10 inlet at different wind speeds. The estimated bias in PM10 concentrations at different wind speeds (2, 8, and 24 km/hr) is less than 3.1%, 6.7% and 13.8% as compared to USEPA's ideal concentrations, and less than -4.9%, -2.8 and 10.4 % as compared to the concentrations calculated by Tolocka et al. (2001), respectively. That is, the measured PM10 is influenced by the wind speed, especially when the wind speed is high. To study the effect of particle overloading, four clean PM10 inlets with grease-coated impaction surface were tested for 5 days sampling. The results showed good comparability ($R^2 > 0.97$) among four inlets. However, the field comparison test of cleaned and uncleaned (not clean daily) PM10 inlets showed that the uncleaned PM10 inlet oversampled PM10 after the first 3-day sampling since particles bounce off from the multiple layers of collected particles on the impaction substrate.

In this research, an oil-soaked glass fiber filter (GFF) supported by an oil-soaked 25-mm porous metal disc was used to replace the grease-coated flat impaction surface of the PM10 impactor to eliminate particle bounce. The laboratory test results showed that the modified PM10 impactor had the same cut-size and sharpness as the original PM10 impactor. The field comparison test of the modified PM10 inlet collocated with cleaned and uncleaned original PM10 inlet is being conducted at National Chiao Tung University, Taiwan. The modified PM10 inlet is expected to eliminate particle overloading during longer sampling period since silicone oil will wick up through the layers of collected particles to reduce particle bounce.

Keywords: PM10, aerosol sampling, particle bounce, particle overloading

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2CM.4

Performance of Compact Cyclones with Taper-Shaped Bodies. PENG WANG, Di Liu, Da-Ren Chen, *Virginia Commonwealth University*

Cyclones have been widely used in a variety of industrial sectors for either removing or recovering particulate matter (PM). It is because of the low cost of machining, operation and maintenance of cyclones. Extended researches have been performed to investigate the performance of cyclones in various geometrical designs. This study introduces a new type of cyclones whose bodies are tapered instead of straight in conventional cyclones. The performance of cyclones with three different contraction angles of 0°, 30° and 60° were experimentally evaluated to study the effect of contraction angle on the cyclone performance. Two experimental setups were used to measure the penetration of particles through the studied cyclones. Polydisperse KCl particles were generated in both experimental setups. In one setup, the large particle aerosol generator (TSI 8180) was used to generate supermicrometer particles, and the optical particle spectrometer (OPS TSI 3330) was applied to measure the particle size distributions both upstream and downstream of studied cyclones. A make-up flow line (with HEPA filter and flow controller) was also included in the setup to vary the cyclone flow rates. In the other setup, a custom-made Collison atomizer was utilized to generate submicrometer particles, and the scanning mobility particle sizer (TSI 3096) was used to measure the particle size distributions both upstream and downstream of studied cyclones.

Our study shows that, the cut-off particle size for each taper-shaped cyclone decreased with the increase of cyclone flow rates. Under the same cyclone flow rate, the cut-off size would decrease with the increase of contract angles. For instance, at the cyclone flow rate of 2 L/min, the cut-off particle size for the cyclone with the 60°-taper-shaped body is ~ 1.7 µm with the pressure drop of 2.26 inH2O, while for the cyclone whose contraction angle is 0°, the cut-off size is ~ 2.6 µm with a pressure drop of 2.14 inH2O. The linear correlation between the dimensionless cutoff particle size and annual flow Reynolds number for studied cyclones was further found in this cyclone study. The regression of the linear correlation could be useful in the future design of cyclones with taper-shaped bodies.

The pressure drop of cyclones at different operational flow rates was also characterized. It is found that the cyclone pressure drop increases quadratically with the operational flow rate for all the studied cyclones. At the same flow rate, the 60°-taper-shaped cyclone has the highest pressure drop and the 0°-taper-shaped cyclone has the lowest drop. On the other hand, it is observed that, among three studied cyclones, the pressure drop of the 60°-taper-shaped cyclone is the lowest for the same cut-off particle size. The above finding implies that cyclones with taper-shaped bodies can effectively remove particles at the lower operational flow rate. Consequently, cyclones with tapered-shaped bodies can save more energy than conventional ones. Because of their compact design, studied cyclones can also be applied as the size-selective inlets for miniature aerosol sensors.

2CM.5

Application of Wet Phase Transition Agglomerator for Synergistic Removal of Fine Particles and Sulfur Trioxide from Stationary Source Flue Gas. Houzhang Tan, Ruijie Cao, Renhui Ruan, Shengjie Bai, XUEBIN WANG, Yongle Du, Hexin Liu, *Xi'an Jiaotong University, China*

A novel technology termed Wet Phase Transition Agglomerator (WPTA) was developed, based on particle growth and agglomeration by heterogeneous condensation, Brownian diffusion, thermophoresis, diffusiophoresis and disturbed pipe flow. The further removal of fine particles and SO_3 from flue gases downstream the wet flue gas desulfurization (WFGD) can be realized by the WPTA in coal-fired power plants.

The WPTA was commercially applied at a 100 MW coal-fired power station unit independently for the first time, after the lab- and pilot-scale experiments and industrial trial cooperating with a wet electrostatic precipitator. It was installed between the WFGD and chimney, and field measurements were conducted to evaluate its performance. The results indicated that the ultra-low emission of particle was realized by the WPTA, and it performed well on SO_3 removal.

The removal efficiency of particles were 53.05% and 71.11%, respectively, at the boiler loads of 90% and 75%. The particle emission was kept below 3 mg/m^3 by the WPTA. Although the concentration of SO_3 was relatively low at the outlet of WFGD due to wet scrubbing, the WPTA could further remove the SO_3 from flue gases. The removal efficiency of SO_3 were 19.29% and 18.87%, respectively, at the boiler loads of 90% and 75%. The SO_3 emission was kept below 2.5 mg/m^3 under all measurement conditions.

Keywords: fine particle; SO_3; growth; agglomeration; simultaneous removal

2CM.6

Evaluation of Particle Loading Performance of Two-stage Filtration System. XINJIAO TIAN, Qisheng Ou, David Y. H. Pui, *University of Minnesota*

Intake air filters are widely used in many industrial sectors to migrate the particles emissions, however, its resistance often increases rapidly and dust holding capacity is low. Installing a pre-filter before the main stage intake air filter is an effective way to improve the filtration performance. Pre-filters are designed to capture large particles before they reach the downstream 2nd-stage filter, which reduce the dust load on the 2nd-stage filter. The pressure drop of the 2nd-stage filter, therefore, increase slowly with extend life-time. In this study, the loading characteristics of a two-stage filtration system, consisting of a 1st-stage pre-filter and a 2nd-stage main intake air filter, is experimentally evaluated. Three different pre-filter media are used on the 1st-stage, and three common intake air filters are used on the 2nd-stage. Bi-modal aerosols consisting of both super-micrometer coarse mode and sub-micrometer fine mode with varied mixing ratios are employed to challenge the two-stage filter system. The influence of pre-filter to the overall performance of the two-stage system will be investigated for different filter combinations, aerosol compositions, and filtration area ratio between the two stages.

2CM.7

Experimental Single Effect Analysis of the Particle Retention Efficiency of a Gas Scrubber. MICHAEL KLAUCK, Kathrin Trollmann, Jeffrey Kobalz, Robin de Winter, Hans-Josef Allelein, *Forschungszentrum Jülich GmbH*

Avoiding or at least minimizing effects of severe accidents in nuclear power plants on the environment is one of the most essential objectives of Severe Accident Management (SAM). A significant part of the fission products released in the process of a loss of coolant accident can reach the containment – the last dense barrier against the leakage of radioactive isotopes – in the form of airborne particles. Once leaked into the atmosphere, gaseous aerosols accumulate over time and might lead to long-term land contamination. Consequently, reliable prediction of aerosol behavior inside the containment during severe accidents is the key to optimizing SAM and thus to minimizing consequences for the environment. This is of particular relevance when it comes to understanding relevant processes regarding particle retention in a water seal (so-called 'pool scrubbing') which is considered to be one of the processes to efficiently filter the containment atmosphere before venting into the surrounding environment.

Several international reactor safety projects have been studying some partial aspects of pool scrubbing and Filtered Containment Venting Systems (FCVS), e.g. OECD/NEA-THAI 3 and the European Commission-funded PASSAM project. However, in order to develop numerical models based on a phenomenological approach, a broad experimental data base with detailed particle characterization is needed. In the framework of the German national 'SAAB' project ('Severe Accident Aerosol Behavior' 2013-2017, funded by the German Federal Ministry of Economic Affairs and Energy), a sophisticated new test facility has been designed and constructed that allows pool scrubbing-related phenomena to be addressed. Its modular set-up allows the investigation of particle retention efficiency at different pool heights up to 6 m and various options regarding injection geometry. Furthermore, two different concepts provide the opportunity to ensure reproducible and constant aerosol generation for both insoluble and soluble particles. Consequentially, the recently launched follow-up SAAB-II project (2017-2021) aims at providing a reliable data base for model development of water-induced particle retention. Pool scrubbing is investigated focusing on single effect tests and the influence of different boundary conditions, including variations of pool height, injection velocity, temperatures, steam supply, particle size distribution, aerosol composition, and injection geometry.

The paper introduces the SAAB-II project and includes a detailed description of the experimental facility, its measurement instrumentation and the aerosol generators, and gives an overview of the experimental results achieved so far.

2CM.8

Effects of Natural and Modified Attapulgite on the Emission of Ultrafine PM and Heavy Metals during Coal Combustion Process. YISHU XU, Xiaowei Liu, Hao Wang, Yufeng Zhang, Minghou Xu, *Huazhong University of Science & Technology*

$PM_{2.5}$ pollution is one of the most severe environmental issues in China. Ultrafine PM is an important part of $PM_{2.5}$ and is of increasing concerns due to its toxicity and control difficulty. Coal-fired power stations are a primary PM source and are facing with increasing strict emission requirements. Currently, devices such as electrostatic precipitators and fabric filters are implemented to capture and remove the PM in flue gas out of the furnace. Although those devices generally have a total PM removal efficiency of as high as 99.9%, they can not effectively capture the ultrafine PM. So, an in-furnace PM reduction technology has been proposed, which is aimed to reduce the formation of ultrafine during the coal combustion process by adding additives into the furnace.

In this study, clay mineral attopulgite (ATT) was selected as the additive. And another two modified ATT were prepared by HCl and CaCl2 treatments of the natural one respectively. Then, the natural and modified ATTs were separately added into pulverized coal and burn in a drop tube furnace at 1500 °C. To explore their impacts on the ultrafine PM formation, the generated PM was collected via a Dekati low pressure impactor and the mass yields, size distributions, compositions and heavy metal contents of the PM were determined via microbalance, XRF and the microwave digestion-ICP/MS procedure.

The results showed that the natural ATT reduced the mass yield of ultrafine PM by ~27%. By the contrast, the HCl and $CaCl_2$ modified ATT reduced the ultrafine PM by ~44% and ~32% respectively, indicating higher ultrafine PM reduction efficiencies than that of the natural one. What's more, Adding ATT reduced the partitioning of heavy metal (e.g., lead, etc.) into the ultrafine PM and this performance was also improved after HCl modification. These results indicated that the above modification treatments could help improve the capture performance of both ultrafine PM and heavy metals.

2IA.1

Impacts of E-Cigarettes Usage on the Air Quality of Vape Shop and Its Nearby Areas. LIQIAO (VICKY) LI, Charlene Nguyen, Yan Lin, Yifang Zhu, *University of California, Los Angeles*

With the rapid growth of e-cigarette (e-cig) market in the U.S, there is an increasing number of independent retail specialty shops (vape shops) that exclusively sell e-cig. The consumption of e-cig in the vape shop might bring a new emission source for aerosol exposure in its indoor environment and nearby businesses. In this study, we selected a representative vape shop in Los Angeles and recorded the number of vaping puffs in every 10 minutes in the shop for four days. Meanwhile, we measured real-time $PM_{2.5}$ concentration and particle number concentration (PNC) in the vape shop as well as its nearby business (~ 3 m away) and outdoor area (~6 m away). Weekly average nicotine concentrations were also measured in each site. The average concentration (SD) of $PM_{2.5}$, PNC and nicotine in the vape shop was 426 (1283) microgram/m^3, 1.89 (2.14)*10^4 /cm^3, and 1.71 microgram/m^3, respectively, which were much higher than those in nearby business (i.e. $PM_{2.5}$: 16.3 (9.3) microgram/m^3; PNC: 8.42 (19.7)*10^3 /cm^3; nicotine: 1.29 microgram/m^3) and outdoor areas (i.e. $PM_{2.5}$: 17.2 (14.0) microgram/m^3; PNC: 8.96 (5.04)*10^3 /cm^3). The number of vaping puffs were significantly correlated with $PM_{2.5}$ concentration (r=0.74, $p<0.001$) and PNC (r=0.71, $p<0.001$) in the vape shop, indicating the significant contribution of e-cig consumption to indoor aerosols. On the day with the highest average puff number, $PM_{2.5}$ and PNC in the vape shop were significantly correlated with those in nearby business and outdoor area ($p<0.05$), suggesting the impacts of vape shop on nearby air quality. Thus, the secondhand emissions of aerosols in the vape shop potentially impacted on both its and nearby indoor environment.

2IA.2

Indoor PM2.5 in an Urban Zone with Heavy Wood Smoke Pollution: The Case of Temuco, Chile. HECTOR JORQUERA, Lupita Montoya, Francisco Barraza, *Pontificia Universidad Catolica de Chile*

Temuco (38°44’ S, 72°36’ W)) is a mid-size city in southern Chile (south of 35° S) with severe ambient air pollution from wood smoke; however, little is known about indoor air quality there. A measurement campaign at 63 households in the Temuco urban area was conducted in winter 2014. Indoor and outdoor (24-hr) $PM_{2.5}$ and its elemental composition were measured and compared. Infiltration parameters and outdoor/indoor contributions to indoor $PM_{2.5}$ were also determined. A statistical evaluation of how various air quality interventions and household features influence indoor $PM_{2.5}$ was also performed. Air sampling was performed at each household only on workdays (Monday through Thursday) for 24 h. A Minivol sampler (TAS, Airmetrics, Eugene, OR, USA, 5 L/min) was installed in each household to collect $PM_{2.5}$ on a Teflon filter (46.2 mm, PTFE, Whatman, NJ, USA). Simultaneously, outdoor $PM_{2.5}$ levels were measured at a single outdoor site using an ambient $PM_{2.5}$ sampler (Partisol 2000i, Thermos, US, 16.7 L/min). Elemental analysis of indoor/outdoor filters by XRF was carried out at ChesterLab (OR, USA). A survey completed by each head of household included questions about household features such as number and type of cookstoves and heaters, whether the household had undergone a weatherization process and presence of pets or smokers.

Median indoor and outdoor $PM_{2.5}$ concentrations were 44.4 and 41.8 $\mu g/m^3$, respectively. An average infiltration factor (0.62 ± 0.06) was estimated using S as a tracer species. Using a simple mass balance approach, median indoor and outdoor contributions to indoor $PM_{2.5}$ concentrations were then estimated as 12.5 and 26.5 $\mu g/m^3$, respectively. Therefore, 68% of indoor $PM_{2.5}$ comes from outdoor infiltration. This high percentage is due to high outdoor pollution and relatively high household air exchange rates (median: 1.06 h^{-1}).

This study found that S, Br and Rb were dominated by outdoor contributions, while Si, Ca, Ti, Fe and As originated from indoor sources. Using continuous indoor and outdoor $PM_{2.5}$ measurements, a median indoor source strength of 75 µg $PM_{2.5}$/min was estimated for the diurnal period, similar to literature results. In the evening period, the median estimate was 135 µg $PM_{2.5}$/min, reflecting a more intense wood burning at night.

Significant (α=0.10) effects of current interventions and household characteristics on indoor air quality were also found. Concentrations in households heated with woodstoves only were higher than those in households that used a mix of heating fuels, supporting the ongoing woodstove changeout program. Weatherized households reduced the infiltration of species of outdoor origin like S, supporting the ongoing subsidized weatherization program; however, indoor $PM_{2.5}$ was not significantly lower in those households, likely due to indoor $PM_{2.5}$ sources offsetting the reduced outdoor infiltration. In households where wood cookstoves were used, indoor $PM_{2.5}$ concentrations were higher than in households using LPG cookstoves, suggesting that a cookstove improvement program may help decrease indoor $PM_{2.5}$. Indoor $PM_{2.5}$ concentrations in smaller subsidized households tended to be higher than in larger dwellings, reflecting an environmental justice issue that needs to be investigated. Overall, this study presents evidence of a complex indoor/outdoor air quality challenge in Temuco — and in southern Chile as well — requiring a continued and diversified management approach. Further, the ongoing slow decrease in outdoor levels means that improving indoor $PM_{2.5}$ in Temuco through ongoing air quality management policies will likely require an extended period of time.

2IA.3

Indoor Aerosols from Home Heating in the Navajo Nation: Sources, Health Effects, and Control. LUPITA MONTOYA, Wyatt Champion, Paul A. Solomon, Kathleen Stewart, Perry Charley, *University of Colorado Boulder*

A previous study determined that using wood and coal for indoor heating in poorly-maintained stoves likely leads to indoor air pollution and negative health effects in the Navajo Nation (NN) (Bunnell et al., 2010). Emissions from residential wood/coal combustion include fine particulate matter ($PM_{2.5}$), which has been linked to respiratory and cardiovascular disease. They suggested that changing indoor heating behaviors and improving heating stove quality would lead to improvements in indoor air quality (IAQ) and health in this community.

Since IAQ in Native Nations in the U.S. has received very little attention, a series of studies were conducted in response to Bunnell's recommendations. First, the In-Home Heating Alternatives Project (IHAP) assessed in-home heating options for residents of the NN (Champion et al., 2017a). This mixed-methods analysis integrated perception, culture, and technical assessments to provide recommendations for a stove replacement program appropriate for this community. Second, controlled experiments were conducted at the University of Colorado Boulder to evaluate emission factors in terms of mass (*mEF*) and energy (*eEF*) for $PM_{2.5}$, organic and elemental carbon (OC, EC), CO and CO_2 for 2 woods and 2 coals commonly used in the NN (Champion et al., 2017b). A third study evaluated potential oxidative and inflammatory effects of $PM_{2.5}$ generated during the combustion of these 4 fuels utilizing an old stove representative of those used in the NN (Li et al., 2018).

Results from IHAP determined that improved stoves, replacement stoves and passive solar heating were viewed most positively by the Navajo; however, replacement stoves showed the best combined results. In particular, replacement stoves that can combust both wood and coal were recommended. IHAP helped uncover areas where community perception, culture, and the technical analyses align and where there are discrepancies necessitating increased dialogue regarding healthier heating methods. It is necessary that community cultural experts (e.g., Diné Policy Institute) conduct thorough cultural assessments to achieve effective integration of culture and science.

The second study determined emission factors for $PM_{2.5}$, OC, EC, CO and CO_2 for the 4 fuels studied. Results showed that Ponderosa Pine had the lowest *mEF* and *eEF* for $PM_{2.5}$, OC, CO and CO_2. Ponderosa Pine also produced about 50% fewer $PM_{2.5}$ emissions than Utah Juniper during the ignition and warm-up phase. Overall, coal compared to wood produced significantly higher emissions on both mass and energy bases.

The third study determined that Ponderosa Pine wood consistently had the strongest oxidative stress and inflammatory effects. PM components, i.e. low-volatility OC, EC, and soluble Cu, Ni and K were positively correlated with the cellular responses. These findings suggest that $PM_{2.5}$ emitted from combustion of wood and coal commonly used by Navajo residents may negatively impact the health of this community.

Together, these studies informed a heating stove intervention in the NN that includes the option of a new USEPA-certified dual (wood/coal) heating stove, designed specifically for the Navajo. We propose that the framework used for this study may be applicable to other Native American Nations, such as the nearby Hopi Nation, where climate conditions and coal use are similar to those of the NN.

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2IA.4

Accuracy of Sensors in Assessing Exposure to Traffic-Related Aerosols. JENNIE COX, Seung-Hyun Cho, Sergey A. Grinshpun, James Ross, Steven Chillrud, Zheng Zhu, Roman Jandarov, Tiina Reponen, *University of Cincinnati*

Traffic-related airborne particles (TRAP) penetrate into buildings affecting the indoor air quality. Improved methods are needed for rapid and accurate assessment of TRAP and the efficiency of control methods. In this study, we evaluated two novel sensors: RTI's Micro Personal Exposure Monitor (MicroPEM) and the MicroAeth real-time black carbon (AE51) sensor. It is recognized in the field that in order to obtain credible real-time measurement results, the data from sensors should be corrected utilizing the information from filter analysis which requires additional time and money. The objective of this study was to create universal correction factors for the MicroPEM and MicroAeth sensors to provide accurate real-time data on PM2.5 and black carbon (BC) in Cincinnati metropolitan area homes, as an alternative to correcting each dataset with the respective filter weights. The two sensors and a PM2.5 impactor (Personal Modular impactor; SKC, Inc.) were collocated in 27 indoor sampling events for 2 days in residences <500 meters from a major roadway and/or had a TRAP score (based on a land-use regression model) of at least 0.33. The PM2.5 impactor samples were analyzed for BC by multi-wavelength integrative sphere method which was gravimetrically calibrated. The real-time PM2.5 concentration from the MicroPEM (RTPM) was averaged and corrected using the gravimetric concentration from the MicroPEM filter. The BC results from the MicroAeth real-time sensor were corrected utilizing BC results from the PM2.5 impactor. Subsets of independent variables in an analysis procedure utilizing multiple linear regression were selected based on lowest Akaike information criterion (AIC). Variables in the model included age and type of building, type of flooring, type of heat (gas or electric), number of smokers, TRAP score, the average daily truck counts within 400 meters, distance to state highways, and distance to a major road (state highways or federal interstates with an average daily truck count of more than 1000). Additional variables of conditions during sampling included season, month, frying food, wood or candle burning, and window opening. The two-day PM2.5 concentrations obtained with the MicroPEM filter ranged from 0.4 to 47.1 $\mu g/m^3$ with a median of 9.5 $\mu g/m^3$. The average correction factor (CF) (MicroPEM filter/RTPM two-day mean) was 1.51 with a coefficient of variation (CV) of 149% (n=27). For the MicroPEM, the final regression model included RTPM values, the average daily truck counts, distance to state highways and distance to federal interstates. By including these variables into the model, the CV was reduced to 40%. The BC values from the PM2.5 impactor ranged from 0.03 to 3.1 $\mu g/m^3$ with a median of 0.4 $\mu g/m^3$. The 48-hour average values from the MicroAeth BC sensor ranged from 0.1 to 2.6 $\mu g/m^3$ with a median of 0.3 $\mu g/m^3$. The average CF (SKC filter/MicroAeth) was 1.3 with a CV of 46% (n=25). Linear regression models considered the variety of variables, but the best model (CV = 49%) did not reduce the CV compared to the correction factor, indicating that these variables are not predictive of indoor concentrations for BC. The poor performance of the models could be due to small sample size and not including other potentially meaningful variables. Still, the PM2.5 model identified three significant factors that indicate the importance of home characteristics for predicting the correction factor. The results from this study will help ensure that the real-time exposure monitors are capable of accurately detecting PM2.5 and BC, which creates the foundation for the further development of user-friendly, field-compatible aerosol instruments for indoor air quality monitoring.

2IA.5

Nanoparticle Resuspension from Surfaces and Resulting Exposures Due to the Use of Consumer Nanosprays in Homes.

RUIKANG HE, Jie Zhang, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

Nanotechnology-enabled consumer sprays are widely used as deodorizers, surface cleaners and for multiple other purposes. These nanotechnology-enabled products release relatively high concentrations of nanoparticles and their agglomerates that may become available for inhalation exposure. This study examined deposition, resuspension, and potential exposures when such nano-enabled sprays are used in a home.

Exposure scenarios examined included adults walking and young children crawling on the floor. The latter was simulated by a robotic crawler. We chose to simulate young children's crawling because their breathing zone is closer to the floor compared to walking. Based on our earlier studies, we selected two Ag-containing and two Zn-containing spray products which generate relatively high mass concentration when applied. The products were applied in a 5 x 9 x 8 ft^3 chamber with controlled background particle concentration. The experiments were performed with carpet and vinyl flooring. Each product was sprayed for 5 min, and particles were allowed to settle on the floor. The particles were resuspended by an adult walking or a robot crawling for 10 minutes every 24 h to determine if resuspension changes over time. Resuspension rate and particle size distributions were measured statically at 0.288 m and 1.1 m above the floor, as well as with a mobile instrument which measured particles in the experimenter's breathing zone during spraying and resuspension. Filter samples were also collected to analyze the morphology and chemical composition of the resuspended particles.

The sprayed particle mass concentration ranged from 0.3 to 58.2 mg/m^3 and the floor-deposited mass density (loading) ranged from 0.00022 x 10^4 to 1.0 x 10^4 mg/m^2. The resuspended particle concentration ranged from 5.2 µg/m^3 to 61 µg/m^3 during walking and from 3.8 µg/m^3 to 9.5 µg/m^3 during robot crawling, depending on the product and floor type. We found that the resuspension rate ranged from 10^{-1} to 10^{-6} h^{-1} and reached a peak value after 24 h for vinyl flooring and after 48 h - 96 h for carpet. As could be expected, the large particles representing agglomerates of sprayed nanoparticle contributed the most to the resuspended particle mass concentration, and small particles were the main contributors to the resuspended particle number concentration. Interestingly, the resuspension rate from the carpet was an order of magnitude higher than that from the vinyl while walking, but only 1.5x higher than that from the vinyl with the robot crawling. Also, the resuspension rate from walking was an order of magnitude higher than that from the robot crawling for both floor types. The resuspended particles and their agglomerates showed the presence of various metals, including Ag and Zn as was advertised in product composition.

Our study shows that when nanotechnology-enabled spray consumer products are used in homes, the sprayed particles not only deposit, but they can also be resuspended from flooring and become available for inhalation exposure. The extent of the resuspension depends on the flooring type, the product, as well as the activity causing the resuspension.

2IA.6

Health Detrimental SVOC Uptake by Infiltrating Ambient Particels Measured with Soot Particle Aerosol Mass Spectrometry. AXEL C. ERIKSSON, Christina Andersen, Anette Krais, Jacob Klenø Nøjgaard, Per Axel Clausen, Aneta Wierzbicka, Joakim Pagels, *Ergonomics and Aerosol Technology, Lund University, Sweden*

Indoor air contains a multitude of health relevant SVOCs originating from active and passive sources. Human exposure occurs continuously, through the relative importance of different exposure routes, some including aerosol particles as intermediate steps, are uncertain. We have studied aerosol particle uptake of a SVOC compound with known adverse health effects; Di(2-ethylhexyl) phthalate (DEHP), from vinyl flooring using in-situ aerosol mass spectrometry. We sampled particles passing through a 1.2 liter aluminum chamber containing 2 dm2 of vinyl flooring with DEHP content of 176 mg /cm3. Mean particle residence times were varied in the interval 1-12 minutes by means of adjusting the flow through the chamber. We used particles infiltrating the aerosol laboratory in Lund for our experiments. We compare our measured aerosol composition with aerosol speciation monitor (ACSM) data from the regional background station Hyltemossa, located approximately 50 km from Lund, in order to separate regional transport from local sources (e.g., particles originating inside the building or city). Furthermore, we injected laboratory generated ammonium sulfate particles for comparison. Our main instrument, used to measure the chemical composition of particles passing though the chamber, was the soot particle aerosol mass spectrometer (SPAMS). We deployed two units in order to investigate the reproducibility of the measurements. We used the "dual vaporizer" mode of SPAMS operation, where the laser vaporizer, which enables soot detection, is periodically disengaged, thus yielding "normal" AMS data intertwined with the SPAMS data. The relative importance of soot containing particles vs non-soot containing particles is thus probed, albeit resulting in non-trivial difficulties in terms of quantification. We used a single particle soot photometer (SP2) to further elucidate the role of soot in the uptake. We used a scanning mobility particle sizer (SMPS) to estimate the surface area available for adsorption. The environmental parameters relative humidity and temperature were monitored. Preliminary results show that the DEHP to total organic aerosol ratio was 5-15% throughout the study period, a total of three weeks. Infiltrating ambient particles were about five times more efficient than laboratory generated ammonium sulfate particles by mass, which we tentatively attribute to increased absorption by the more abundant organic aerosol fraction. Infiltrating particles include a serendipitous event with transported wildfire emissions from the Iberian peninsula (in October 2017), approximately 3000 km upwind our experiment. In addition, there were several events where organic aerosol originating from renovations of the building housing the laboratory was sampled, and what appears to be fresh traffic emissions occurring in the immediate vicinity of the fresh air intake supplying the laboratory. We find that aerosol mass spectrometry is a suitable tool to study the process of health detrimental SVOC uptake by aerosol particles, even in the comparatively clean (PM1 is typically below 5 µg/m3) laboratory air. It is our aim to add more health relevant compounds besides DEHP to coming investigations.

2IA.7

Managing Indoor Air Quality in ClimACT Schools. Susana Marta Almeida, Patrice Blondeau, Vitor Manteigas, Joana Lage, Ana D'Espiney, Marina Almeida-Silva, Nuno Canha, VÂNIA MARTINS, Tiago Faria, Karla Gonçalves, José Luís Alexandre, Ricardo Chacartegui, Jesus Lizana, José António Becera, Ana Gamarra, Yolanda Lechon Perez, Amaia Fernandes, *C2TN, IST, Universidade de Lisboa, Portugal*

The indoor environment of schools where students stay for long periods of time is a matter of primary concern due to the vulnerability and sensibility of children to air pollutant exposure. This work aims to assess the Indoor Air Quality in 38 ClimACT schools located in the Sudoe region of Europe and generate guidelines for a proper management of the schools.

Within the scope of the Interreg Sudoe ClimACT project, Indoor Air Quality audits were performed in 2 classrooms of 38 schools from Portugal, France, Spain and Gibraltar. Levels of PM10, PM2.5, CO2, CO and TVOC were measured with portable direct reading instruments. Passive sampling of volatile organic compounds (benzene, toluene, styrene, tetrachloroethylene, trichloroethylene, m-xylene, o-xylene, p-xylene, 1-4 dichlorobenzene, α-pinene) and aldehydes (formaldehyde, acetaldehyde, acrolein, propanal, butanal, pentanal, isopentanal, hexanal, benzaldehyde) were carried out with Radiello® diffuse tubes. Measurements were performed during one week from Monday to Friday.

PM10, PM2.5, CO_2, TVOC and formaldehyde frequently exceed the guidelines of 20 µg/m^3, 10 µg/m^3, 2250 mg/m^3, 600 µg/m^3 and 30 µg/m^3, respectively. The mean indoor levels of these pollutants ranged as follows: PM10 - 0.04-99 µg/m^3; PM2.5 - 0.03-41 µg/m^3; CO_2 - 882-4381 mg/m^3; TVOC - 0-854 µg/m^3; formaldehyde - 0.10-91 µg/m^3.

The PM10 concentrations measured during the occupied periods were higher than in non-occupied showing that occupancy, through re-suspension of previously deposited particles and possible particle generation, influences the indoor levels of airborne particles. Concentration peaks for TVOC were identified during cleaning activities and during occupied periods due to VOC emissions by occupants (biogenic VOCs, body lotions, etc) and students' activities. Higher CO_2 levels were observed during students' activities inside the classrooms. Even causing negative effects on the students' performance, CO_2 is not classified as a pollutant by the World Health Organization. However, it can be considered a good proxy of insufficient ventilation in classrooms. Therefore, CO_2 can be used to alert teachers to open windows due to the poor air quality or to adjust the amount of outdoor ventilation in Heating, Ventilating and Air Conditioning Systems.

In order to reduce student's exposure to pollutants in classrooms a proper ventilation strategy need to be adopted. Such strategy is even more important in naturally ventilated schools where the air exchange rate is only based on the manual airing of classrooms.

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2IA.8

MakerSpaces: An Emerging Indoor Aerosol Exposure Source. Anthony Ramos, Justin Keller, Tim Raymond, DABRINA DUTCHER, *Bucknell University*

MakerSpaces (or HackerSpaces) are facilities with shared tools designed to allow people and groups to come together with the purpose of fabricating devices and sharing ideas. These facilities have increased in popularity in recent years. They are increasingly common in community spaces such as libraries and schools, ranging from elementary schools to universities. Pre-existing spaces, which were not originally designed to be used as MakerSpaces, are sometimes adapted to be a MakerSpace with little consideration of the ventilation system. Tools in these spaces are quite varied ranging from laser cutters to 3-D printers to soldering irons and sewing machines. Many of these tools are known to produce particles, but there is little information available on their impact on the air quality in these spaces. Three MakerSpaces were monitored at Bucknell University with a Scanning Mobility Particle Sizer while tool use was recorded. Each of these facilities is outfitted with different tools and different ventilation system characteristics. Observed particle number concentrations ranged from background level to more than 300,000 particles per cubic centimeter, depending on ventilation rates and tool use. The most significant recommendation stemming from these observations is that MakerSpaces with tools that can be operated remotely (such as 3-D printers and Laser cutters) are not suitable for ventilation systems triggered by occupancy sensors.

2IM.1

Inversion of Scanning Electrical Mobility Spectrometer and SMPS Measurements. RICHARD FLAGAN, Yuanlong Huang, Amanda Grantz, *California Institute of Technology*

The Scanning Mobility Particle Sizer, (SMPS) enables rapid particle size distribution measurements, but the data obtained as the voltage is scanned are analyzed using the transfer function for a constant voltage DMA; that transfer function would be valid for plug flow (uniform velocity within the DMA), but boundary layers within the DMA cause particles to follow different trajectories through the classification region, altering the transfer function. Particles also experience a distribution of time delays between the times when they exit the DMA and are counted by the CPC. Convolution of a delay-time distribution function with the DMA transfer function has been used to invert SEMS/SMPS data, but the distortions caused by the DMA itself are not taken into account. Recent coupling of finite element simulations of the flows and fields within the scanned DMA with Brownian dynamics simulations of the advection, migration, and diffusion of particles during SEMS measurements have revealed additional deviations of the transfer function from that at constant voltage.

Prompted by these results, we have re-examined SEMS/SMPS data inversion, which requires: (i) a transfer function for the instrument; (ii) a model that will be used to represent the resultant particle size distribution function; and (iii) an algorithm that will be employed to solve the inverse problem to deduce the size distribution that best represents the collection of signals acquired during the measurement. At constant voltage, the physics-based, Stolzenburg model of the transport and diffusion of particles within the DMA accurately describes the instrument. The delay time distribution caused by can be approximated the residence time distribution from one or more so-called continuously-stirred tank reactors combined with a fixed delay. The new transfer function for the TSI long-column DMA reveals a delay-time distribution within the classification region, and a more complex downstream delay time distribution that the previous models suggest. Combined with empirical transmission and detection efficiency functions and theoretically predicted charge distributions, these refinements reproduce the time and size variation in particle transmission through and detection by the SEMS/SMPS measurement system and form the foundation for data inversion. The computational effort to obtain the real-instrument transfer function is, however, large. We have, therefore, undertaken the development of a theoretical transfer function for the scanned-voltage DMA analogous to the Stolzenburg transfer function for the static DMA, and that is more readily applied to other DMA operating conditions, and to different DMA designs.

The discretized form of the particle size distribution also strongly affects the data inversion. Multimodal lognormal distributions impose a potential shape bias on the size distribution. Representation as a set of discrete particle sizes (delta functions) or as a histogram representation are also commonly used. Linear splines are used in a number of algorithms. Higher order basis functions can also be used. The degree of approximation directly impacts the quality of the data fit obtained. The algorithms employed can also affect the quality of the inversion. In this study, we examine the sensitivity to different models for the same instrument, size distribution representations, and inversion algorithms in order to understand their effects on the recovered distributions. While the focus of this study has been on SEMS or SMPS data inversion, the results have implications for all methods used to determine aerosol particle size distributions.

2IM.2

Improving the Accuracy and Precision Of Sub-10 nm Atmospheric Nanoparticle Measurements with a New High Flow DMPS. JUHA KANGASLUOMA, Lauri R. Ahonen, Tiia M. Laurila, Runlong Cai, Joonas Enroth, Stephany Mazon, Frans Korhonen, Pasi Aalto, Markku Kulmala, Michel Attoui, Tuukka Petäjä, *University of Helsinki*

Measurement of atmospheric sub-10 nm nanoparticle number concentrations has been of substantial interest recently, which, however, is subject to considerable uncertainty that has not been examined thoroughly. We report a laboratory characterization of a high flow differential mobility particle sizer (HFDMPS), which is based on the SEADM Half-mini type differential mobility analyzer (DMA) and Airmodus A11 nano condensation nuclei counter, and show the first results from atmospheric observations from Hyytiälä, Finland during spring of 2017. The HFDMPS utilizes the state-of-the-art aerosol technology, and is optimized for particle size distribution measurements in the sub-10 nm size range by a moderate resolution DMA, optimized and characterized low-loss particle sampling and minimal dilution in the detector.

We analyze the performance of the HFDMPS in two aspects: the instrument is analyzed in terms of the PtQ value, which directly connects the instrument performance to the number of counted particles. PtQ is shown to be useful parameter is determining the instrument detection limit and, when combined with the DMA sizing resolution, measurement uncertainties.

Further, we present an exhaustive laboratory calibration to the HFDMPS and compare the inverted atmospheric particle number concentrations to the long-term size segregated aerosol number size distribution measured with the Hyytiälä long-term DMPS. Because of the optimized sampling and higher sensitivity of the HFDMPS, it detects about two times more 3-10 nm particles than the long-term DMPS, and by having better counting statistics by a factor of 3.5-9 depending on the size, the counting uncertainties are reduced about 50% as compared to the long-term DMPS. The HFDMPS did not observe any sub-2.5 nm particles in Hyytiälä, and the reason for that was shown to be the inability of DEG to condense on such small biogenic particles, instead of lack of sensitivity. Last, we discuss the general implications of our results to the sub-10 nm DMPS based measurements.

2IM.3

Characterization of the Boosted 3776 Butanol TSI CPC in the Sub 2 nm Range. Activation of Sub 2nm Particles with Butanol.

MICHEL ATTOUI, *LISA Paris Est Creteil University France*

Boosted butanol laminar sheathed condensers CPCs have (Kuang2012) demonstrated their ability to detect sub 3 nm with acceptable detection efficiency although lower than mixing cpc with di ethylene glycol as working fluid. In the other hand Kangasluoma et al. 2015 have showed than unsheathed condensers butanol CPCs are able to detect particles down to 1 nm. So if unsheathed condenser can detect particles of 1 nm why not the sheathed condenser CPC design? The abilities of this CPC in terms of flowrates control (sheath and capillary) are used to study the activation (or no activation) of THABr and TBABr monomer by lowering the aerosol losses in the capillary and working at the limit or threshold of the homogeneous nucleation.The presentation gives the effect of the flowrate in the capillary on the detection efficiency for different temperatures difference DTs between the saturator and condenser until the limit of the homogeneous nucleation. The figures 1 and 2 below give the inverse mobility spectra of TBABr (tetrabutylammonium bromide) with flowrates of 50 cc/min 70 cc/min in the capillary at the limit of the homogeneous nucleation and respectively in the condenser. The figures 3 and 4 give the results with THABr (tetraheptylammonium bromide) in the same with 50 et 70 cc/min aerosol flowrate in the capillary at the limit of the homogeneous nucleation always.

Keywords: CPC, detection efficiency, nanoparticles

2IM.4

Penetration Efficiency of Sub-3 nm Particles in the Sampling Line of an Electrical Mobility Size Spectrometer. YUEYUN FU, Mo Xue, Runlong Cai, Juha Kangasluoma, Jingkun Jiang, *Tsinghua University*

Due to the high diffusivity of sub-3 nm particles, their diffusion loss through the instrument sampling line is large. In addition, the often used Gormely-Kennedy (G-K) formula for penetration efficiency through a straight cylindrical tube may fail for sub-3 nm particles. The G-K formula is an asymptotic analytical solution of the convection diffusion equation and is applicable when particle concentration at the inlet is uniform. However, the boundary conditions used to derive the G-K formula are usually violated in practical use, especially for sub-3 nm particles. In addition, when the flow field changes in the sampling line, particle concentration will redistribute in the cross-sectional profile that may result in larger concentration gradient near the wall and thus additional particle loss. Thus, penetration efficiencies through three-way connectors, elbows, bends, and core-sampling tubes can be different from values predicted by the G-K formula. Experiments and numerical simulation were performed to study the penetration efficiency of sub-3 nm particles through the sampling line of an aerosol electrical mobility spectrometer. Straight cylindrical tube, elbow, three-way connector, and core-sampling tube were characterized. The penetration efficiency through a soft X-ray neutralizer and a DMA were also evaluated. Strategies to improve the sampling efficiency of sub-3 nm particles were tested. For instance, properly designed core sampling tube (2 LPM core-sampling flow, 8 LPM transport flow, 60 cm in length) can increase the sampling efficiency of 1.5 nm particle by 26%, comparing to a straight cylindrical tube with the same length and total flow. The penetration efficiencies through each parts of the spectrometer sampling line were integrated together to properly recover size distributions of sub-3 nm particles.

2IM.5

A Modified Real-Time Method to Measure Particle Geometric Surface Area with a Time Resolution of 1s. LIPENG SU, Qisheng Ou, Leo N.Y. Cao, David Y. H. Pui, *University of Minnesota*

This paper reports the improvement of a real-time method to measure geometric surface area (GSA) of nanoparticles with a higher precision and an improved time resolution of 1s. In this method, a unipolar diffusion charger was used, followed by two identical systems in parallel, both consisting of an ion trap and an electrometer. By applying different voltages on the two ion traps, charged particles with different electric mobility may penetrate through the corresponding ion trap, with the carried charges measured by the electrometer downstream. The two measured electric currents were combined in a biquadratic subtractive process to achieve linear correlation with GSA of nanoparticles precisely. To validate the newly developed method, laboratory tests and field measurements were carried out by combined measurement using above-mentioned system and a Scanning Mobility Particle Sizer (SMPS) simultaneously. Good agreements were found between the two sets of instruments, with the improved unipolar charging technique having better time resolution of 1s.

2IM.6

Aitken's Condensation Counter: Bringing History to Life. DYLAN LEIGH-MANUELL, Suresh Dhaniyala, *Clarkson University*

John Aitken, a late 19th century meteorologist, physicist, and engineer, began his research into condensation and phase transformations in 1875. In 1890, this research led to the development of the Aitken dust counters, considered to be the first condensation nuclei counters. Because of their small size, simplicity, and ability to generate reproducible measurements, Aitken's dust counters, the pocket dust counter in particular, became widely used for the next half a century. This presentation outlines how John Aitken's early condensation nuclei counters were able to optically count particles in the air. We will also describe the process taken to restore an original Aitken Portable Dust Counter along with an original Aitken Pocket Dust Counter to working order. Lastly, we test the two historical counters and compare their performance in measuring aerosol concentrations to modern day instruments.

2IM.7

Application of Size-Independent Charging of Nanoparticles for Improving DMA-Classification Performance. Yoohyun Ock, Jeonggeon Kim, Mansoo Choi, DONGGEUN LEE, *Pusan National University*

The goal of this study was to achieve a significant improvement in the size-selection performance of DMA, by combining unipolar charging and the condensational method of growing nanoparticles. We developed a size-independent unipolar charger consisting of a saturator, a condenser, a corona charger, and an evaporator. Starting with a two-fluid mixing design, a porous-alumina-lined saturator was tested in terms of the size uniformity of particles after their condensational growth in a subsequent condenser. 20-nm Ag and 65-nm NaCl polydisperse nanoparticles were successfully grown into droplets of few micrometers with a geometric standard deviation of 1.20 or less. A simple model was also developed to explain the heat and mass transfer occurring in the saturator and condenser, resulting in predictions of particle growth that agreed with experimental results. The entire charging system was experimentally evaluated in terms of size dependencies of charging efficiency and charge numbers. The results revealed that ~52% of the nanoparticles were uniformly charged with a charge number of +32, irrespective of the particle sizes. A regular nano DMA, using the proposed size-independent charging system in place of a bipolar charger, was finally tested to determine its productivity when size-classifying particles. It was found that the proposed charger was eight times more efficient for DMA size selection compared to the bipolar charger, and became more advantageous as the target particle size decreased. These promising results were reconfirmed by TEM image analysis of the produced monodisperse particles.

2IM.8

A Versatile Portable Exhaust Particle Sampling System to Extend Particle Number Measurements below 23 Nanometers. MARKUS BAINSCHAB, Alexander Bergmann, Panu Karjalainen, Jorma Keskinen, Jonathan Andersson, Athanasios Mamakos, Tero Lähde, Christoph Haisch, Oriana Piacenza, Ananias Tomboulides, Zisimos Toumasatos, Leonidas Ntziachristos, Zissis Samaras, *Graz University of Technology*

Modern and near-future combustion engine vehicle technology may emit notable levels of particles below the current particle size threshold (23 nm) of the European Particle Number (PN) emission standards. The Horizon 2020 funded project DownToTen (DTT) is developing a sampling and measurement methodology to characterize exhaust aerosol emissions down to at least ten nanometers. This study presents the first prototype of a portable exhaust particle sampling system (PEPS) developed in the framework of the project.

Laboratory experiments, in which various dilution systems were challenged with aerosols from a variety of sources, showed that a double porous tube dilution (PTD) system is the method offering the lowest detectable size. The radially inflowing dilution air in a PTD reduces thermophoretic and diffusional losses of <23 nm particle sizes and the compact all-metal design facilitates the realization of a heated dilution stage. The first porous tube is supplied with hot (350°C) dilution air. The second PTD operates at room temperature. Dilution may be combined with different conditioning chambers, depending on purpose: an aging chamber to thermodynamically stabilize aerosol, an evaporation tube or a catalytic stripper to isolate non-volatile particles, or a photo-oxidation chamber to address secondary aerosol formation. Sample flowrates and dilution ratios settings are controlled by mass flow controllers.

The system is characterized with laboratory and real exhaust aerosols in terms of particle losses and dilution ratio stability. Computational fluid dynamics (CFD) simulations provide detailed insights on the air flow through the porous medium, and the mixing of the dilution air and the sample flow. Further, the propagation of pressure pulses and their impacts on the dilution ratio is examined. Two different laboratory experiments were conducted to validate the pressure pulsation results of the CFD simulations. The first uses an aerosol source with a controllable pressure level, and uses pressure sensors with high temporal resolutions at various spots in the dilution system to show how pressure pulsations affect the dilution ratio and the performance of downstream particle number measurement devices. The second experiment uses an ultrasonic transit time flow meter to inspect the sample flow downstream of the porous tube diluter to check for high frequency flow fluctuations predicted by the simulations. Finally, the sampling system is employed for engine exhaust measurements on a chassis dynamometer.

The comparison of the developed dilution system with the commercial measurement systems fulfilling current EU PN Regulation demonstrates the feasibility of the DownToTen PEPS for sub 23 nanometer engine exhaust particle number measurements. The versatile tests with laboratory particle sources and the measurements of vehicle exhaust particles suggest that DTT PEPS extends the exhaust particle measurement range down to 10 nm and below reliably.

2IN.1: INVITED

Ice Nucleating Particle Properties Relevant to Aerosol Cloud Interactions in the Himalaya Region. Shweta Yadav, Rebecca Venezia, Ryan Paerl, MARKUS PETTERS, *North Carolina State University*

The foothills of the Himalaya mountains are often blanketed by a thick haze layer that originates from anthropogenic and natural sources. There is a dearth of data on ice nucleating particle (INP) concentrations within these airmasses, thus limiting modelling studies that try to assess the influence of INPs on ice cloud formation. Here we present new data on INPs measured from filter and precipitation samples collected in rural and urban locations of northern India, including the states of Jammu & Kashmir, and Himachal Pradesh. In addition, we characterize the INP properties of mineral dust samples obtained from the Thar Desert, which is located in the northwestern part of the Indian subcontinent. Ice nucleation activity was obtained using the cold-stage technique. For the ambient samples, fluorescent particle size and concentration were determined using multi-wavelength flow cytometry. Factors that influence INP concentrations are explored. Results show that rainwater-derived INP concentrations are similar to the lower bound of observations obtained over the North American continent. Strong signals from pollution or bioaerosol were not evident. Ice nucleation active site density of Thar Desert dust, normalized by the geometric surface area of the aerosol, was similar for mobility-selected sizes ranging from 200-600 nm. Furthermore, the Thar Desert dust is well described by parameterizations that were built from dust data collected elsewhere around the globe. These data suggest that local pollution is not a strong source of INPs over the northern Indian subcontinent. Furthermore, existing dust parameterizations can be applied to estimate INP concentration if information about suspended dust surface area is available.

2IN.2: INVITED

Influence of Heterogeneous Ice Nucleation of Sea Spray Aerosol on Southern Ocean Clouds. CHRISTINA MCCLUSKEY, Paul DeMott, Thomas Hill, Kathryn Moore, Sonia Kreidenweis, Ruhi Humphries, Alain Protat, Greg McFarquhar, Susannah Burrows, Andrew Gettelman, *National Center for Atmospheric Research*

Clouds occurring over the Southern Ocean (SO) are often comprised of supercooled liquid and are abundant, with an annual average cloud fraction greater than 0.8. Global climate models fail to simulate SO cloud phase and lifetime, leading to large Southern Hemisphere energy biases in climate model simulations. It is hypothesized that these shortfalls are due to poor numerical representations of ice phase transitions and ice microphysics. In a series of observational and modeling studies, we have characterized ice nucleating particle (INP) populations over the SO and investigated their role in primary ice nucleation and subsequent cloud glaciation in a global climate model.

Two methods were used to determine immersion freezing INP number concentrations (n_{INPs}); 1) the ice spectrometer, an offline immersion freezing technique and 2) the continuous flow diffusion chamber, an online INP measurement. These two methods were deployed onboard the Australian Marine National Facility RV Investigator as part of the Clouds, Aerosols, Precipitation, Radiation and atmospherIc Composition Over the southeRN ocean (CAPRICORN) voyage from March to April in 2016. These data represent the first survey of INPs over the SO region in over four decades. Extraordinarily low n_{INPs} were observed in this unique region, with no more than 1 INP active at -30 °C per liter of air. Using the atmospheric component (community atmospheric model, CAM5) of the DOE Community Earth System Model with implementation of a physically-based parameterization for sea spray organic aerosol, simulations using nudged meteorology were conducted for the CAPRICORN study period. Modeled aerosol mass, number and composition were used as input for various parameterizations proposed for predicting n_{INPs}. Estimates of n_{INPs} were in agreement with field observations and results demonstrated that a recent empirical marine INP parameterization may be used to predict observed concentrations of nINPs from the CAPRICORN project.

These new observational constraints and a marine INP parameterization allow for modeling studies to investigate the influence of INPs and primary ice nucleation on cloud phase in SO clouds. As such, the NCAR community atmospheric model (CAM5) will be used in a series of sensitivity simulations designed to explore different representations of INPs and subsequent primary ice nucleation. Simulated cloud occurrence and phase will be directly compared to ship and aircraft based observations, including comprehensive measurements of aerosol and cloud properties, made during the Southern Ocean Clouds, Radiation, Aerosol Transport Experimental Study (SOCRATES) from January to February 2018.

2IN.3: INVITED

Surface Chemistry of Ice Nucleating Mineral Dust Particles. ALEXEI KISELEV, Alice Keinert, Alexei Nefedov, Weijia Wang, Christof Woell, Thomas Leisner, *Karlsruhe Institute of Technology*

Heterogeneous ice nucleation on the surface of mineral dust particles is an important process responsible for the ice formation in atmospheric clouds. Recently, the surface topography and crystalline structure have been recognized as the two major factors defining the ice nucleation efficiency of K-feldspar, a very common aluminosilicate mineral abundant in the atmosphere as a universal component of airborne mineral dust particles. However, the chemistry of the mineral surface in contact with supercooled water or ice remains poorly characterized due to the lack of experimental methods sensitive to the water-mineral interface. Several questions have to be answered to complement the picture of heterogeneous nucleation, such as the importance of surface charge, the role of framework cations, protonation state of the mineral surface, and the role of ionic species dissolved in water.

In this contribution, we address some of these questions by conducting water freezing experiments on the well-defined surfaces (thin sections) of alkali feldspars with various crystallographic orientations. We show how their freezing efficiency can be predictably modified by treating the surface by argon plasma of different density. We further investigate the chemical composition of the samples in the environmental scanning electron microscope (ESEM) by means of X-ray energy and wavelength dispersive spectroscopy (EDS and WDS), as well as with ultra-high vacuum IR adsorption spectroscopy and X-ray photoelectron spectroscopy (XPS). The measurements conducted with these surface sensitive analytical methods allow us to make certain conclusions about the role of surface chemistry and the particular importance of hydroxyl groups in the nucleation of ice on mineral surfaces. Moreover, these findings offer a possibility of bridging the gap between the atomistic simulations and laboratory experiments, with the ultimate goal of creating a molecular dynamic model of heterogeneous ice nucleation on realistic substrates.

2IN.4

Mineral Dust Aerosol Measurements throughout the Global Free Troposphere and Implications for Cirrus Formation.

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Lab and field studies indicate that mineral dust particles are efficient ice nuclei, and recent airborne measurements confirm the dominant role of dust on cirrus cloud formation in the northern hemisphere. However, the net climate impact of mineral dust is not well constrained in part due to the lack of dust abundance measurements above the Earth's surface. We present new airborne mineral dust measurements from the 2016-2017 NASA ATom (Atmospheric Tomography) campaigns that cover the entire Pacific and Atlantic basins from the boundary layer through the free troposphere. This global dataset fills a critical measurement gap for dust in the background upper troposphere. Measured concentrations are compared to global simulations of dust aerosol, with a focus on model accuracy at cirrus altitudes. We identify source contributions to the remote troposphere and examine mechanisms of vertical transport and removal. Using heterogeneous nucleation efficiencies from laboratory studies, we estimate that background dust particles can contribute to cirrus formation throughout wide regions of the global upper troposphere. In particular we explore north-south hemispheric gradients of dust aerosol and the implications for differences in cirrus properties.

2IN.5

Immersion Freezing Efficiency of Airborne Mineral Dust at Various Particle Size-classes. NAAMA REICHER, Shira Raveh-Rubin, Yinon Rudich, *The Weizmann Institute of Science*

Mineral dust is a prominent atmospheric aerosol, affecting clouds microphysics and climate by its ability to act as cloud condensation nuclei (CCN) or as ice nucleating particles (INP). Mixed-phase clouds, which contain both supercooled droplets and ice crystals, are highly sensitive to the presence of INPs since they can trigger instant glaciation. It is still not well understood how nucleation is facilitated by the dust surface, but it was shown that mineralogy plays a crucial role in determining the efficiency of the ice nucleation process. Feldspars, for instance, were identified recently as highly efficient INPs, compared with other abundant mineral phases, such as clay minerals (illite, montmorillonite and kaolinite), calcite or quartz. Moreover, different types of feldspars also differ in their ice nucleation efficiency and active temperature regions. Therefore, the prediction of ice nucleation efficiency of different dust events depends on the mineral composition of the dust, which can vary according to the geographic source of the dust, the particle size and changes in its mineralogy during atmospheric transport. In order to examine the effect of the particle size on ice nucleation efficiency in ambient samples, airborne mineral dust was sampled during dust events from two source regions, the Sahara Desert and the Syrian Desert. The particles were collected and size-segregated using micro-orifice uniform deposit impactor (MOUDI) during five dust storm events. The collected particles were immersed in nL-size water droplets using microfluidics technique, and ice nucleation properties were studied using the WeIzmann Supercooled Droplets Observation on Microarray (WISDOM). We found that ice nucleation efficiency was similar for the different dust sources, but varied with particle size. In all but one event, the freezing efficiency of larger particles was higher, and supermicron particles exhibited higher ice nucleation efficiency in comparison with the submicron particles. Moreover, active site density spectra (ns) of supermicron particles were similar to the spectra obtained for standards of feldspar minerals, suggesting that this size fraction is more characterized by feldspars. In the event where particles size did not affect the ice nucleation efficiency, the total efficiency was lower than that measured in the other dust events, and this was attributed to a nearby biomass-burning event, which contributed biomass-burning aerosols to the sample or interacted with the mineral dust surface. These results suggest that mineralogy change with the particle size and that further characterization of the mineralogy difference with atmospheric transport is needed to better establish our prediction of ice nucleation efficiency of atmospheric dust.

2IN.6

Effect of Mineralogy, Particle Size, and Composition on the Immersion Freezing Properties of Three Central American Volcanic Ashes. LEIF JAHN, Daniel Williams, Michael Polen, William Fahy, Ryan Sullivan, *Carnegie Mellon University*

Ash generated from explosive volcanic eruptions represents a large source of material periodically injected into the atmosphere. Recent studies have suggested that volcanic ash is a potentially significant source of ice nucleating particles (INP). However, the current body of research regarding how the chemical composition of volcanic ash relates to its ability to nucleate ice is lacking, especially in atmospherically relevant particle size ranges. In this work, we analyzed three volcanic ash samples collected in the vicinity of recent volcanic eruptions (Volcàn de Fuego, Guatemala, 2015; Santiaguito, Guatemala, 2011; Soufrière Hills, Montserat, 2011). Each of the samples were sieved to a <37 µm size fraction, and the Fuego sample was further separated into <2.5 µm, 2.5-10 µm, and 10-37 µm fractions using a custom dust generator and MOUDI sampler. X-ray diffraction (XRD) analysis indicates that the ashes are mostly composed of Na- and Ca-rich feldspars, as well as varying amounts of silica polymorphs and pyroxenes. Additionally, XRD was used to quantify the amount of amorphous non-crystalline material, which likely has weak ice nucleation ability. Freezing properties were examined in the immersion mode using a droplet freezing cold plate. Analysis of the droplet freezing temperature spectra shows that the ashes contain efficient INP in the range of -10 to -25 °C that are consistent with the presence of feldspars—some of the most ice-active mineral phases. The Fuego ash sample demonstrated freezing ability comparable to that of some of the most ice-active K-rich feldspar samples reported in the literature, which we attribute to the presence of Na-rich/K-poor anorthoclase feldspar. Additionally, smaller particle sizes were observed to be more ice-active, even when accounting for differences in particle surface area. Ash elemental composition at the population level was examined through ion chromatography, and individual particle elemental distribution and morphology was examined through scanning electron microscopy. Our results indicate that these volcanic ash aerosols can be a significant source of INP and that this freezing ability is driven by the crystalline phase content, mineralogy, and quantity of feldspar minerals in the ash.

2IN.7

Ice-Nucleating Properties of Coal Fly Ash Particles in Cirrus Cloud Conditions. NSIKANABASI UMO, Robert Wagner, Romy Ullrich, Kristina Höhler, Naruki Hiranuma, Amanda Lea-Langton, Harald Saathoff, Alexei Kiselev, Peter G. Weidler, Heike Wex, Sarah Grawe, Jenny M. Jones, Alan Williams, Benjamin Murray, Thomas Leisner, Ottmar Möhler, *Karlsruhe Institute of Technology*

Globally, over 600 Tg of coal fly ash (CFA) are produced annually from coal combustion for industrial and domestic energy production. A certain proportion of these aerosol particles is emitted to the atmosphere and may impact air quality, human health, and radiative transfer through the atmosphere. Coal fly ash can also modify cloud microphysical and optical properties, hence influencing the climatic and the hydrological cycles. However, our understanding of the role of CFA in nucleating ice at conditions relevant to cirrus clouds is lacking and requires research efforts. Here, we investigate the ice-nucleating properties of CFA, obtained from four different sources, in the deposition mode at the AIDA (Aerosol Interaction and Dynamics in the Atmosphere) cloud simulation chamber. All the CFA samples (particle median diameter ~ 0.6 µm) showed significant ice nucleation activity at ice saturation ratios between 1.04 and 1.38 evaluated at the maximum relative humidity with respect to ice reached during each experiment, in the temperature range from 214 K to 251 K. The ice nucleation active surface site densities of these particles in the deposition mode were estimated between 10^9 - 10^{11} m^{-2} within the same temperature coverage of the experiment. One of the CFA samples studied in this work showed high ice nucleation activity at even lower ice saturation ratios (1.04 - 1.16) at ~ 228K, which suggests that pore condensation and freezing may be the dominant ice formation mechanism as there was no corresponding high activity of this particular CFA in the immersion freezing mode. The results from this study have clearly established that CFA aerosol particles efficiently nucleate ice in the deposition mode. Future study should focus on probing the factors driving their ice-nucleating abilities. CFA particles may contribute to cloud ice formation, in particular, close to the source region where these particles are emitted directly into the atmosphere. Also, future modelling and experimental studies are needed to further investigate and assess the abundance of CFA aerosols and their contribution to cloud ice formation on regional and global scales.

2IN.8

Characteristics of Ice Nuclei in the North China based on Mountain Measurements. KAI BI, Xincheng Ma, Fei Wang, Yunbo Chen, Ping Tian, Quan Liu, Delong Zhao, Gavin McMeeking, Ezra Levin, *Beijing Weather Modification Office*

Ice nuclei measurements were conducted at Haituo Mountain in northwest Beijing in 2016-2017 winters. The characteristics of wintertime ice nuclei particles (INPs), as well as their relation with meteorology elements and atmospheric aerosols were investigated with a continuous flow diffusion chamber (CFDC) and a Bigg mixing cloud chamber. Relationships between pollutants and IN number concentrations were also studied. The results showed that the concentration of Ice nuclei particles(INPs) active at -10℃~-25℃ typically ranged from 0.2#/L~64.8#/L with Bigg Chamber. The INPs active at -15℃~-35 ℃ at water supersaturation 5% ranged from 0.5#/L~362.4#/L with CFDC. The INPs active at -25 ℃ and water supersaturation -5%~5% were from 2.5 #/L ~54.9 #/L. The relationship of INPs and T match the exponential distribution, as f(T)=0.0016583*exp(-0.43353*T). INPs did not increase obviously in heavy polluted days comparing to clean days. The INPs increase after snow in 2/3 of snow cases. Of all meteorological elements, wind speed and airflow direction appeared to influence IN number concentrations.

2MS.1

A Facile Aerosol-based Synthesis of Cu-Ce-O Hybrid Nanoparticles for Synergistic Catalysis of Methane Combustion.

DE-HAO TSAI, *National Tsing Hua University*

The synergistic effect of Cu-Ce-O hybrid nanostructure has shown the promise for catalytic methane combustion. Here, we aim to develop an aerosol-based two-stage thermal treatment method to (1) synthesize the Cu-Ce-O hybrid nanoparticle (NP) with a tunable oxidation state directly in gas phase, and (2) provide a mechanistic understanding of surface reduction of the Cu-Ce-O hybrid NP for catalysis of methane combustion. After evaporation-induced self-assembly followed by a thermal decomposition (i.e., 1st stage) to form metal oxide NP at the 1st stage thermal treatment, a temperature-programmed, aerosol-based hydrogen reduction process was employed for direct tuning the oxidation state of the NP in the gas phase (the 2nd stage thermal treatment). Differential mobility analysis, x-ray diffractomery, x-ray photoelectron spectroscopy, and scanning electron microscopy were employed complementarily for characterization of particle size, morphology, crystallinity, elemental composition, and oxidation state of the NPs. The results show a successfully catalysis on methane combustion over various initial oxidation states of Cu through the hybridization with ceria . The results show a high activity with a low light-off temperature, a high light-off stability and operation stability toward catalytic methane combustion. The prototype method is especially useful to fabricate a variety of nanocatalysts with different oxidation states of active metals by design for the study of methane-based energy and environmental applications.

2MS.2

Measurements and Simulations of Nanomaterial Formation and Gas Phase Intermediates' Behavior in Buoyancy Opposed Flame Synthesis Reactor. IGOR RAHINOV, Johannes Sellmann, Sebastian Kluge, Hans Juenger, Alexey Fomin, Matthieu Raphael Lalanne, Sergey Cheskis, Christof Schulz, Hartmut Wiggers, Andreas Kempf, Irenaeus Wlokas, *The Open University of Israel*

Production of the iron oxide nanoparticles with tailored properties by flame-assisted synthesis should rely on detailed understanding of the mechanisms governing their formation and nucleation from the gas phase. Specifically, nanoparticle formation in flames is strongly influenced by the residence-time–temperature history inside the flame [1,2]. We study how the temperature history can be intentionally modified by orienting flames either in an upward-firing or downward-firing configuration. We also investigate the influence of unintended residence-time modifications caused by sampling nozzles. These phenomena are investigated by experiments and simulations for the synthesis of iron oxide nanoparticles from premixed iron-pentacarbonyl-doped hydrogen/oxygen flat flames[3,4]. The experiments apply molecular-beam sampling with a particle mass spectrometer to measure particle sizes and a quartz microbalance to detect the presence of condensed matter [5]. Laser-Induced Fluorescence (LIF) and Intracavity Laser Absorption Spectroscopy (ICLAS) were applied to monitor gas-phase Fe and FeO, respectively[4,6,7]. The simulations rely on a finite-rate chemistry approach with detailed diffusion, particle dynamics are described by a bi-modal population balance model. The results revealed a strong impact of the reactor orientation on the velocity field. It is demonstrated that the downward-burning flame forms a detached stagnation point, causing longer residence times at elevated temperature than an upward- or horizontally firing flame, permitting the growth of larger particles. These iron oxide particles are eventually formed in the recombination zone of the flame, but no condensed matter was found in the reaction zone. In presence of a probing nozzle, the overall shape of the flame changes, depending on the distance of the probe from the burner dramatically. The corresponding residence times are also strongly affected by the probe. Due to strong stagnation effects the 1-D model cannot be applied directly to this "nominally flat" flame configuration. Rather, the experimentally determined Fe and FeO concentrations were compared to outputs of detailed reaction mechanisms in one-dimensional models using the previously determined flow field. This allowed to draw suggestions for further optimization of iron-chemistry mechanism.

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2MS.3

Synthesis of Crumpled Graphene Nanostructures Decorated with Multicomponent Metal Nanoparticles in a Flame-driven High Temperature Reducing Jet Reactor. MOHAMMAD MOEIN MOHAMMADI, Santosh Srivatsa Gunturi, Shikuan Shao, Raymond Buchner, Mark Swihart, *University at Buffalo - SUNY*

Among carbonaceous materials, graphene has become attractive because of its unique properties such as high specific surface area, good electrical conductivity, flexibility, and high mechanical strength. The most common synthesis method of graphene is based on graphite oxidation to graphene oxide (GO) followed by thermal or chemical reduction of GO to reduced graphene oxide (rGO). In thermal reduction methods, a small amount of GO is typically placed in a high temperature inert or reducing environment for a specific time. In addition, to improve certain properties or to add new features, rGO is decorated with other compounds which usually requires additional synthesis steps. Here, we demonstrate the continuous single-step synthesis of three-dimensional crumpled graphene (CG) nanostructures decorated with multicomponent metal nanoparticles including CG-cobalt-nickel and CG-iron-cobalt-nickel using the High Temperature Reducing Jet (HTRJ) process. In this process, combustion products of a fuel-rich hydrogen flame pass through a converging-diverging nozzle. An aqueous solution or dispersion of precursors injected at the throat section of the nozzle is atomized by the hot high-velocity gas stream. The resulting droplets evaporate in reducing environment containing excess H_2. After the reaction zone, products are cooled immediately and collected on a filter paper. The key advantage of the HTRJ system over common flame-based aerosol synthesis methods is the separation of flame and product formation zones, which allows synthesis of nanomaterials that can be reduced by H_2 in the presence of H_2O. We have utilized the capabilities of this system to synthesize CG nanostructures using an aqueous dispersion of GO as the precursor. Moreover, by adding nickel, cobalt, and ferric nitrate salts to the GO precursor solution, we decorated CG nanostructures with iron-cobalt-nickel nanoparticles of less than 10 nm average diameter. The HTRJ process is a potentially scalable, continuous synthesis method of CG and CG-metal nanostructures. The nanostructures made by this process can be used in electrocatalysts for fuel cells, electrodes in batteries and supercapacitors, conductive inks for printed electronics, and in many other applications where a graphitized carbon-metal nanomaterial is needed.

2MS.4

Tailored Synthesis of Macroporous Pt/WO3 Nanoaggregates via Flame Spray Pyrolysis and Their Photocatalytic Properties. OGI TAKASHI, Ghana Rinaldi Febrigia, Tomoyuki Hirano, Kikuo Okuyama, *Department of Chemical Engineering, Hiroshima University*

A high surface area is a key feature of nanoparticles, and enhances their performances in many applications, including photocatalysis. However, handling nanoparticles is more difficult than handling micron- or submicron-sized particles. It has been reported that exposure to large amounts of nanoparticles over a long time period can harm human health and the environment. One strategy for addressing this issue is nanostructuration of micron- and submicron-sized particles, which gives the desirable properties associated with nanoparticles (e.g., high surface area and low density) and improved handling properties. In this research, high-surface-area macroporous WO_3 nanoaggregates particles with deposited Pt (Pt/WO_3) were successfully synthesized using flame spray pyrolysis. The macroporous structure was tailored by changing the mass ratio of the polystyrene template to ammonium tungstate pentahydrate. The cavities between the nanoaggregates formed mesopores, which increased the surface area. The high surface area resulting from meso- and macro-pores in the synthesized Pt/WO_3 particles improved their photocatalytic activities in visible-light-induced photodegradation of rhodamine B. The combination of a high surface area and the presence of an in situ-deposited Pt cocatalyst gave a high photodecomposition rate, approximately 9.6 times higher than that achieved with dense WO_3 particles. This research provides a promising strategy for synthesizing submicron particles with high surface areas at a high production rate, and is suitable for industrial applications.

2MS.5

Flame Aerosol Integrated Role-To-Role Lamination Technique for High Performance Battery Fabrication Procedure.

LUTZ MÄDLER, Michael Gockeln, Robert Kun, Suman Pokhrel, *University of Bremen, Faculty of Production Engineering*

$Li_4Ti_5O_{12}$ (LTO) lithium-ion-batteries with high energy density, efficiency and long life time are powerful sources of energy. However, their main drawback is the large scale production cost both in terms of the material designing and the fabrication procedure. Today, the complex and labor-intensive industrial battery fabrication includes coating slurry-based electrodes, assembly and life-cycle test. Hence, to develop next generation innovative battery technology, new synthesis-fabrication procedures are necessary to ensure excellent performance and reduced cost.[1] In our recent work, single and/or double flame aerosol syntheses were utilized to obtain active LTO material and transfer the particles in the dry state on the battery substrate using role-to-role lamination technique.[2] During double flame aerosol combustion, (1) a single individual flame was used to obtain LTO (2) second individual flame was used to obtain carbon.[3] The two aerosol streams were mixed at a certain point above the flame to obtain homogenous C-LTO mixture. For the single flame synthesis, LTO (without carbon) was sprayed on the collecting unit placed at 60 cm above the flame followed by layer transfer either to the standard and/or flexible substrates using role-to-role laminator. The active material and layers were characterized using XRD, BET, and TEM imaging. The carbon content in the active material was determined using thermogravimetric analysis and Raman spectroscopy. The results of the laminated battery electrodes showed enhanced specific discharge capacities compared to reference electrodes prepared using conventional slurry-based doctor blading technique. The variation in lamination pressure was a key to enhanced electrochemical performance. The solvents and/or binder free layer fabrication technique is expected to become economic and promising technique for its use in the flexible and/or non-flexible substrates in the future.

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2MS.6

High Throughput Screening of Precursor-Solvent Combinations for Flame Aerosol Chemistry to Design Phase Pure Li4Ti5O12 Energy Storage Materials. SUMAN POKHREL, Florian Meirhofer, Haipeng Li, Johannes Birkenstock, Michael Gockeln, Robert Kun, Lutz Mädler, *University of Bremen, Faculty of Production Engineering*

The industrial development of lithium-ion-batteries based on advanced energy storage materials such as $Li_4Ti_5O_{12}$ (LTO) relies on the phase pure material. Flame aerosol technology for the production of such materials is a key to such synthesis. While the chemistry of the impurity free energy storage material synthesis depends on the choice of precursor-solvent combinations, systematic investigation of lithium and titanium precursors dissolved in five different organic solvents were screened followed by flame aerosol combustion.[1,2] The results of the precursor-solvent screening showed rapid stabilization of humidity sensitive precursors in highly combustible organic acids inhibiting prior TiO_2 precipitation in the solution. The physicochemical properties of aerosol derived particles were extracted using XRD/Rietveld refinements, thermogravimetric analysis, mass spectrometry and vibrational spectroscopy. The results of the LTO particles obtained from the aerosol combustion of highly miscible precursor-solvent combinations with the absence of prior formation of colloidal particles resulted in ultrafine and single crystalline nature with primary particle diameters ranging 4-9 nm. The flame aerosol combustion of less-stable precursor-solvent combinations inducing prior TiO_2 precipitation produced much larger particles and high TiO_2 content reducing LTO phase to as low as 34%. The overall results showed direct relationship between the stabilities of the precursor-solvent chemistry on the nanoparticle properties. To study the energy storage capacity, the pure phase LTO particles were coated on the battery substrates using doctor blading technique. The results of the battery performance showed discharge capacity of 146.5mAh/g for 450 cycles at 1C with the charge retention of 85%, revealing high rate and efficient charge reversibility.

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2MS.7

Electrospray Atomization and Deposition of Nanoparticle Suspensions Leading to Nanostructured Porous Coatings.

JOSE L CASTILLO, Santiago Martin, Daniel Rodriguez-Perez, Francisco J Higuera, Pedro L Garcia-Ybarra, *Universidad Nacional de Educacion a Distancia - UNED*

The controlled deposition of aerosols is a valuable tool to prepare thin nanostructured porous coatings as required in many applications. Thus, aerosol nanoparticles can be used as building blocks for materials synthesis leading to thin porous layers with a prescribed morphological structure and still retaining a large surface/volume ratio as distinctive feature. Coatings formed by the accumulation and adhesion of incoming aerosol nanoparticles acquire a morphological structure controlled by the form of the constitutive particles and by the way in which these particles arrive and attach to the forming material. A proper control of the aerosol particle dynamics may lead to granular deposits with a well-prescribed bulk morphology and surface structure.

Experiments have been conducted to prepare nanostructured materials from the steady electrohydrodynamic atomization of liquid suspensions. The electrospray is kept in the cone-jet mode with a Taylor cone at the needle exit and a very thin jet emerging from the cone tip. At some distance away from the cone tip, the jet breaks up into a spray with droplets much smaller that the needle radius, forming a cloud with a narrow distribution of tiny charged droplets. The droplets are driven by the electric field and evaporate along their path leaving a solid residue of charged nanoparticles which are collected on a substrate. The range of parameters leading to a stable cone-jet was studied for two different suspensions; carbon nanoparticles in ethanol and catalytic inks formed by Pt supported on carbon nanoparticles and Nafion® in ethanol.

The morphology of the deposits has been examined by means of digital scanning electron microscope (SEM) images. Upper views of the deposit show a layer structure based on clusters of nanoparticle agglomerates formed by the attachment at the deposit of nanoparticles coming from several electrospray droplets, with the cluster size (of the order of 10 microns) increasing with the flow rate. Lateral SEM images of the deposits cross-sections were processed to calculate the deposit mean density and porosity. The porosity is rather high (always larger than 90%) decreasing as the electrospray flow rate increases.

Coatings prepared from catalytic inks were tested as electrodes in a fuel cell. The performance of the electrodes synthesized using different values of the electrospray flow rate was studied. The electrodes have shown extremely large specific power (reaching a power of 21 kW per gram of Pt in the cell) due to the outstanding properties of the electrosprayed catalytic layer: large porosity, uniform distribution of the catalyst and high density of (Pt) active sites.

These results for fuel cell electrodes show the advantages of the electrospray method in a particular case. But the same methodology could also be used for other applications. The structure of the synthesized material can be tailored according to the application needs to have a given porosity and surface composition. Moreover, layered or composed materials (with a different porosity or different composition on each layer) can be prepared by adequate changes in the control parameters (liquid flow rate and applied voltages in the electrospraying technique) which determine the dynamics of the particles approaching the deposit.

2MS.8

Aerosol Particle Restructuring: Molecular Dynamics of High Aspect Ratio Carbon Nanotubes. NIKOLAOS KATERIS, Adam M Boies, *University of Cambridge*

The Floating Catalyst Continuous Vapour Deposition (FCCVD) process for carbon nanotube (CNT) production is extensively used, but the kinetics within the process are poorly understood. The process involves injection of methane, ferrocene, and thiophene into a hydrogen filled reactor, downstream of which CNT aerogel is continuously drawn. Individual CNTs grow on catalyst nanoparticles, which form after the decomposition of thiophene and ferrocene. The CNTs then collide and form bundles. Further collisions of the bundles lead to the formation of the aerogel. This work aims to explain the mechanism of aerogel formation.

The collision frequency of CNTs has been investigated through stochastic simulations [1]. These simulations allow the calculation of the collision rates of straight and curved CNTs. The specific purpose of this work is the determination of the realignment rate of CNTs and CNT bundles, in order to examine the aerogel formation criteria. This is achieved with a spatially adaptive mesoscale molecular model.

The molecular dynamics after collision are governed by intermolecular van der Waals forces and the time evolution of the molecule arrangement is calculated on LAMMPS. The mesoscale model performs Langevin Dynamics calculations within a simulation box. A bead-spring model is employed to model the axial and bending stiffness of CNTs. Intermolecular forces are modelled using a Lennard-Jones potential, with its parameters scaled according to Markus Buehler's 2006 paper [2], in order to account for the discrete nature of the beads.

It is observed that the bead spacing affects bundling time and using the conventional value of bead spacing equal to CNT diameter is excessively computationally expensive. Therefore, in order to simulate bundling of long CNTs, a mesoscale model of spatially adaptive resolution is developed. This novel approach to bead-spring modelling involves maintaining fine beads in areas where intermolecular forces are dominant and modelling the rest of the molecule with coarse beads. The simulation is regularly paused and the CNT length is repopulated by beads of resolution that provides the necessary accuracy in critical regions.

These modelling techniques enable the calculation of bundling rates of individual CNTs and CNT bundles. For instance, re-alignment time of two individual CNTs is in the order of 1 ns (for lengths of order of 100 nm), whereas their collision time is of the order of up to 100 ns, for a wide range of CNT lengths. Long CNTs and CNT bundles have slower re-alignment rates, which approach collision rates. This re-alignment data is vital for the understanding of the aerogel formation process. Multiple CNTs can also be placed in a simulation box to collide and form bundles, and eventually an aerogel, thus giving information about the critical values that enable aerogelation to occur.

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2RA.1

Aerosol Enhancement in the Tropical Tropopause Layer Controlled by Deep Convection, In Situ Production, and Mixing. SHANG LIU, Pengfei Yu, Troy Thornberry, Andrew Rollins, Yuyan Cui, Karen Rosenlof, Ru-Shan Gao, *University of Colorado, Boulder*

Aerosols in the tropical tropopause layer (TTL) are of great interest as the TTL is the main gateway for material transport from the troposphere to the stratosphere. Understanding the abundance and distribution of aerosols in this pristine region is also important for quantification of the anthropogenic influence on climate. However, our knowledge of aerosol properties in the TTL is limited. To bridge this gap, we measured vertically-resolved aerosol size distributions in the TTL over the western Pacific warm pool, an area that features deep tropical convection due to the warm sea surface. The measurements were performed using a custom-built optical particle counter onboard the NASA WB-57F as well as weather balloons based at Guam (13.5º N, 144.8° E) during the NASA POSIDON (Pacific Oxidants, Sulfur, Ice, Dehydration, and cONvection) campaign in October 2016.

From 9 research flights and 1 balloon profile, we find that the vertical distributions of aerosol in the tropical troposphere over Guam can be described by three layers, each with distinct vertical structure and properties. The first layer is from the surface to 5 km, in which the aerosol mass mixing ratio (MMR) decreased logarithmically with height from 2 ppb to 0.08 ppb. The second layer ranges from 5 km to 13.5 km, with the latter coinciding with the typical height of the tropical convective outflow. Aerosol concentrations in this layer are very low, with an average MMR of 0.07 ppb. These observations suggest that aerosols in this layer have been efficiently removed by convection, which serve as an effective aerosol sink by scavenging. The TTL constitutes the third layer, ranging from 13.5 km to 19 km. In the TTL, the aerosol MMR increases linearly with altitude from 0.07 ppb to 1.2 ppb. Good correlation of aerosol MMR with O3 in the TTL indicates that inmixing of the aerosols from the stratosphere may play a role in the rapid increase of aerosol mass. The increase of aerosol MMR could also result from particle growth due to in situ chemical production at the outflow of tropical convections. A global sectional aerosol model coupled with the Community Earth System Model has been used to examine the relative contribution of vertical mixing and local formation of the aerosol mass. In addition, a Lagrangian particle dispersion model (FLEXPART) has been used to identify the source regions of the TTL aerosols and their precursors. In summary, our results demonstrate multiple controls of the tropical deep convection in the life cycle of aerosols, acting as a sink for lower-altitude aerosols and an indirect source of aerosols in the upper troposphere and lower stratosphere.

2RA.2

Physico-chemical Properties of Free Tropospheric Particles at the Remote Pico Mountain Observatory, in the Azores.

CLAUDIO MAZZOLENI, Lynn Mazzoleni, Paulo Fialho, Swarup China, Bo Zhang, Andrea Baccarini, Kaelan Anderson, Simeon Schum, *Michigan Technological University*

To better model the effects of atmospheric particles on climate, it is essential to further our understanding of their lifecycle and their interactions with clouds and radiation; this is particularly critical for understudied remote regions of the atmosphere, such as the marine free troposphere. To this end, we studied the properties of atmospheric particles from the elevated Pico Mountain Observatory (2225 m.a.s.l.), in the Azores, Portugal. The station typically lays above the low marine clouds and samples free tropospheric air masses that are transported over the North Atlantic Ocean from North America or are recirculated from North Africa. For the last several summers, we have measured at the site the atmospheric particle light scattering coefficients using a 3-wavelength nephelometer, the particle concentrations using a two-channel optical particle counter, and the black carbon equivalent mass and iron-containing dust concentrations with a 7-wavelength aethalometer. In addition, we collected samples on different media to study their chemical composition, and the single particle morphology and ice nucleation properties. We used retroplume simulations from the FLEXible PARTicle dispersion model (FLEXPART) to interpret the results based on the air mass origin, transport path, transport time, and source type and region.

We studied the physico-chemical properties of the atmospheric particles, including their optical properties, the detailed bulk chemical composition, and the individual particle morphology and their elemental composition. In this presentation, we will focus in particular on the properties of particles collected during episodes dominated by the transport of mineral dust to the site. Using scanning electron microscopy coupled with energy dispersive X-ray spectroscopy, we performed mineralogical analysis of individual dust particles and studied the heterogeneity of different elements within each particle. These properties are relevant to the particles' interactions with clouds and radiation, especially owing to the location of the atmospheric particles sampled at the station, typically above the marine clouds.

2RA.3

The Birthplace of Cloud Nuclei - A Global Perspective from the Atmospheric Tomography Mission. CHRISTINA WILLIAMSON, Agnieszka Kupc, Anna Hodshire, Jack Kodros, Jeffrey R. Pierce, Pengfei Yu, Karl D. Froyd, Eric Ray, Frank Erdesz, Mathews Richardson, Thaopaul Bui, Charles Brock, *NOAA ESRL and CIRES, University of Colorado Boulder*

Atmospheric aerosols affect climate by direct scattering of solar radiation and by altering cloud properties. Current uncertainties in anthropogenic aerosol forcing are one of the largest factors in total uncertainties in predicting climate change. In situ measurements of the properties, origins and climatic relevance of aerosols are needed to constrain global climate models, validate satellite measurements and better understand aerosol sources and processing in the atmosphere. In-situ measurements of aerosol in the remote free troposphere have hitherto been particularly sparse.

The Atmospheric Tomography Mission (ATom) is a unique set of measurements characterizing the remote free troposphere. ATom uses the NASA DC-8 as a flying lab, equipped with gas phase and aerosol measurements, flying over both Pacific and Atlantic Ocean basins, with near pole-to-pole coverage, constantly scanning between 0.2 and 13km altitude. Measurements are conducted in all four seasons to capture seasonal variations.

We describe the measurement of aerosol size distributions from 3 to 3000nm diameter on ATom, how these measurements inform our understanding new particle formation in the remote atmosphere, and how these particles influence climate. We compare these contiguous global datasets of size distributions ATom with output from two global models with online aerosol microphysics: GEOS-Chem-TOMAS and CESM-CARMA.

2RA.4

Measurements of Black Carbon Concentration and Aerosol Light Absorption during the Finokalia Aerosol Measurement Experiment (FAME-16). ANTONIOS TASOGLOU, Kalliopi Florou, Evangelos Louvaris, Aikaterini Liangou, Georges Saliba, Spyros Pandis, *Carnegie Mellon University*

A month of continuous air monitoring took place at the Finokalia Atmospheric Observatory in Crete, Greece during the summer of 2016. No significant human activities occur within 15 km of the station. The sampled air masses originated from the Balkans, northern Africa and the Mediterranean Sea. This study focused on the measurement of the aerosol light absorption in a remote area characterized by highly oxidized organic aerosol and also high sulfate levels.

In addition to a high-resolution Aerosol Mass Spectrometer (HR-ToF-AMS) and a Scanning Mobility Particle Sizer (SMPS) for size distributions and chemical composition measurements, a suite of instruments for the measurement of the light absorption and the refractory black carbon (rBC) mass concentration was deployed. This included an aethalometer, a photoacoustic extinctiometer (PAX_{405}), a Multi-angle Absorption Photometer (MAAP), and a Single Particle Soot Photometer (SP2).

The fine aerosol mass concentration ranged from 0.3 to 8 $\mu g\ m^{-3}$, with the sulfate and organics accounting for almost 80% of the total mass. The organic aerosol was quite oxidized with an average O:C equal to 0.7. The rBC concentration ranged from 0.04 to 0.3 $\mu g\ m^{-3}$, representing from 2 to 15% of the fine aerosol mass. The measured light absorption was two or more times higher than that of fresh BC. Mie theory was used to evaluate if the effect of the coatings of BC cores by organics and sulfate could explain this absorption enhancement. The role of brown carbon and also other non-BC light-absorbing material was investigated. A thermodenuder was used to link the volatility of the organic aerosol with the observed BC absorption enhancement.

2RA.5

Blowing Snow Influences on Aerosol Composition: Insights from Bulk and Single Particle Measurements in Coastal Antarctica. MICHAEL GIORDANO, Anita Avery, J. Doug Goetz, Lars Kalnajs, Kerri Pratt, Nathaniel May, Alex Lee, Peter DeCarlo, *Drexel University*

In the cryosphere, many open questions regarding aerosol production, processing, transport, and lifetimes still exist. Recent evidence suggests that blowing snow may significantly alter these aerosol processes on both local and regional scales but real-time, on-line evidence is scant. This presentation focuses on both bulk composition changes and single particle results from deploying a suite of instruments, including an aerosol mass spectrometer (AMS), to the Antarctic sea ice during the 2ODIAC campaign, with a focus on blowing snow events. Bulk measurements of the supermicron aerosol and blowing snow samples show that ion ratios are overall consistent with seawater ion ratios, contrary to the submicron ion ratios which show enhancements in sea salt (Na and Cl) concentrations. In the submicron aerosol, these bulk composition changes are shown to be independent from air mass origins. Furthermore, in the snow, no evidence of bromine production is observed indicating that these important reactions are likely occurring in the aerosol scale. Additionally, single particle results from the AMS show a variety of chemical species in addition to sulfates in the submicron aerosol mass. K-means cluster analysis also shows distinct changes in the overall aerosol mass spectra during to blowing snow events.

2RA.6

Arctic Aerosol Sources: Results of PMF on PM10 Collected at Ny Ålesund. GIULIA CALZOLAI, Silvia Nava, Massimo Chiari, Franco Lucarelli, Fabio Giardi, Silvia Becagli, Rita Traversi, Mirko Severi, Laura Caiazzo, David Cappelletti, Stefano Crocchianti, *University of Florence and INFN Florence, Italy*

Ny Ålesund is located on a western fjord of Svalbard Islands, in the northernmost point influenced by the warm West Spitsbergen Current, and thus it is an ideal site for the study of the interaction between the climate change and the atmosphere, ocean and land variations. At the Gruvebadet laboratory, samplings are ongoing since 2010 in the period March to September; in particular, in this work we focus mainly on the results gained by the analysis of daily PM10 samples collected during the 2015 campaign.

Daily PM10 samples were analyzed for the ionic composition by Ion Chromatography (IC) and for metals and rare earth elements (REEs) by Inductively Coupled Plasma - Atomic Emission Spectroscopy (ICP-AES). Further, for the first time, daily samples collected in 2015 were analysed for the elemental composition by Particle Induced X-ray Emission (PIXE) analysis. PIXE is an almost unrivaled technique for the characterization of mineral dust, as it is sensitive to all the crustal elements (except O), including Si, which is usually not accurately quantifiable with other common chemical techniques.

Data on PM10 concentrations and speciation will be shown, for the year 2015 and in comparison with previous years. Further, preliminary data on the 2016 campaign will be also shown: in such year, a new sampling method was set up in order to enhance the sensitivity of the PIXE technique.

Source apportionment was performed by applying the Positive Matrix Factorization (PMF) model. PMF allowed the identification and the quantification of the contributions to the aerosol burden of several sources such as sea salt, ammonia sulfate, biomass burning, mineral dust, nitrate, anthropic/arctic. Contributions vary in the range from few percent (e.g., biogenic emissions) to almost 50% for sea salt. The 2015 campaign was particularly interested by biomass burning transport episodes from Northern America.

The backward trajectories of air masses produced through HYSPLIT software were used to identify regional source areas for the identified PMF factors/sources. This analysis was used to strengthen the interpretation of each factor as a physical source as well as to gain further information on the aerosol long-range transports.

The logistic assistance of the Polar Support Unit of the CNR Department of Earth and Environment (POLARNET) is gratefully acknowledged.

2RA.7

Global Long-range Transport and Lung Cancer Risk of Polycyclic Aromatic Hydrocarbons Shielded by Viscous Secondary Organic Aerosols. MANISHKUMAR SHRIVASTAVA, Sijia Lou, Alla Zelenyuk, Richard Easter, Richard Corley, Brian Thrall, Philip Rasch, Jerome Fast, Staci L. Simonich, Huizhong Shen, Shu Tao, *Pacific Northwest National Laboratory*

Polycyclic aromatic hydrocarbons (PAHs) have toxic impacts on humans and ecosystems. One of the most carcinogenic PAHs, benzo (a) pyrene (BaP), is efficiently partitioned to and transported with atmospheric particles. Laboratory measurements show that adsorbed BaP degrades in a few hours by heterogeneous reaction with ozone, yet field observations indicate BaP persists much longer in the atmosphere, and some previous chemical-transport modeling studies have ignored heterogeneous oxidation of BaP to bring model predictions into better agreement with field observations. We attribute this unexplained discrepancy to the shielding of BaP from oxidation by coatings of viscous organic aerosol (OA). Accounting for this OA viscosity-dependent shielding, which varies with temperature and humidity, in a global climate/chemistry model brings model predictions into much better agreement with BaP measurements, and demonstrates stronger long-range transport, greater deposition fluxes, and substantially elevated lung-cancer risk from PAHs. Model results indicate that the OA coating is more effective in shielding BaP in the mid/high latitudes compared to the tropics because of differences in OA properties (semi-solid when cool/dry vs. liquid-like when warm/humid). Faster chemical degradation of BaP in the tropics leads to higher concentrations of BaP oxidation products over the tropics compared to higher latitudes. This study has profound implications demonstrating that OA strongly modulates the atmospheric persistence of PAHs and their cancer risks.

2RA.8

Adsorption of Trace Atmospheric Gases in Atmospheric Boundary Layer by Dust Aerosol Particles Emitted from Arid Source Areas. BORIS KRASOVITOV, Tov Elperin, Itzhak Katra, Andrew Fominykh, *Ben-Gurion University of the Negev, Israel*

Scavenging of active trace gases by mineral dust storm aerosols is a result of gas adsorption. Adsorption of trace atmospheric gases such as NO_2, SO_2 and HNO_3 by dust aerosol particles contributes to the evolution of concentration distribution of the trace constituents and can affect subsequent chemical reactions in the atmosphere. In this study we suggest a two dimensional model of adsorption of trace atmospheric constituents by mineral particulate matter emitted from area source in a desert. The model is based on the application of theory of turbulent diffusion in the atmospheric boundary layer (ABL) in conjunction with the model of gas adsorption by porous solid particles. The analysis is focused on the local spatial scale (10 km), which is the most important for dust entrainment into the atmosphere. The numerical model is formulated using parametrizations based on the aeolian experiments. Aeolian field experiments were performed at a dust source site (loess soil in Northern Negev, Israel) using a portable boundary layer wind tunnel to determine the emitted PM fluxes for different wind speeds and varying soil conditions. For individual wind-erosion events, wind shear produced turbulence near the surface is responsible for particle entrainment into the atmosphere, while turbulence in the atmospheric boundary layer affects particle diffusion and deposition. Therefore the wind velocity profiles used in the simulations were fitted from our data previously obtained in field measurements conducted in the Northern Negev (Israel) using the experimental wind mast. Size distribution of the emitted dust particles in the numerical simulations was taken into account using a Monte Carlo method. We determined numerically concentration distributions of the particulate matter and trace gas based on the values of shear velocity and emitted dust flux from the soil measured in experiments. Analysis was performed for the meteorological conditions typical for the Northern Negev region. The obtained results demonstrate that using parametrizations based on direct field measurements of wind profile and aeolian erosion has a potential to reduce the uncertainties in atmospheric particulate matter transport and trace gases distribution models and provides a more realistic assessment of dust and trace gases concentration distributions. The model enhances our capacity of quantification of atmospheric dust effects in climate models as well as health risk assessment. The results of the present study can be useful in an analysis of different meteorology-chemistry models including adsorption of trace atmospheric gases by dust aerosol particles emitted from arid source areas.

3AC.1

Not Fade Away: Photolytic Brown Carbon Formation in Aqueous Aerosol. DAVID DE HAAN, Devoun Stewart, Tobin Gramyk, Alexia De Loera, Duncan Ugland, Christian Carmona, Antonio Rojas, *University of San Diego*

Based on results from bulk aqueous phase lab experiments, it is now commonly assumed that brown carbon formed by small, water-soluble aldehydes + ammonium salts are quickly destroyed by sunlight. However, recent cloud chamber studies showing more intense browning with solar simulator lights turned on suggest that this common assumption does not apply to evaporating aqueous aerosol, where brown carbon is more likely to be formed by radical polymerization pathways. Here, we present results of small-chamber and steady-state aerosol experiments where we quantify the amount of brown carbon formed as a function of UV or sunlight exposure and other variables. In deliquesced ammonium sulfate aerosol at 50% RH, we find that 90 min of sunlight destroys brown carbon formed by methylglyoxal + methylamine dark reactions. However, if hydrogen peroxide is added as an OH radical source, more brown carbon is formed in sunlight than in dark reactions (with or without hydrogen peroxide), further evidence of rapid photolytic brown carbon production. We will report on studies of additional chemical systems that form brown carbon, including glyoxal + SO_2.

3AC.2

Enhanced Formation of Brown Carbon Particles at Low Relative Humidity. Masao Gen, Dandan Huang, CHAK K. CHAN, *City University of Hong Kong*

Reactions between dissolved ammonia, $NH_{3(aq)}$, and carbonyls can form light-absorbing species in atmospheric particles. According to previous research, such reactions can be accelerated by actively removing water from the reaction system. Here, we examine the effects of relative humidity (RH) on the reactive uptake of glyoxal (Gly) by aqueous particles of ammonium sulfate (AS), ammonium bisulfate (ABS), sodium sulfate, magnesium sulfate, ammonium nitrate (AN), and sodium nitrate (SN) at RHs of 30, 45, 60, and 75%. In-situ Raman analysis was used to quantify particle-phase Gly via the ν(C-H) peak at 2900-3050 cm^{-1} and a colored product, 2,2'-biimidazole (BI), by its broadband fluorescence as a function of uptake time. The presence of BI was verified by off-line UV-vis and fluorescence characterization, as well as surface-enhanced Raman spectroscopy measurements. Overall, the Gly uptake rate increases with decreasing RH, reflecting the "salting-in" effect, but is suppressed for SN particles at 30% RH, probably due to increased particle viscosity resulting from the formation of Gly oligomers. For $NH_{3(aq)}$-containing particles, the BI formation rate increases significantly with decreasing RH or aerosol liquid water (ALW); however, the BI formation rate is negligible for crystalline AS particles at 30% RH and ABS particles under all RH conditions due to extremely low $NH_{3(aq)}$. Compared to that at 75% RH, the BI formation rate is enhanced by factors of 2.9×10 at 60% RH and 3.3×10^2 at 45% RH for AS particles and 6.5×10 at 60% RH, 2.1×10^2 at 45% RH, and 4.6×10^2 at 30% RH for AN particles. These enhancement factors are much larger than those estimated from increased reactant concentrations due to decreases in RH and ALW alone. We postulate that the reduction in ALW at low RH increases the Gly uptake rate via the "salting-in" effect and the BI formation rate by facilitating dehydration reactions.

3AC.3

Effect of Relative Humidity on Light Absorbing Secondary Organic Aerosol Formation. NETHMI KASTHURIARACHCHI, Alex Lee, *National University of Singapore*

The uptake of water-soluble volatile organic compounds into aqueous aerosol, fog and cloud droplets can result in subsequent aqueous-phase reactions producing secondary organic aerosols (SOA). Glyoxal (Gly), an α-dicarbonyl compound formed by the oxidation of isoprene and aromatic compounds, is extensively studied as a precursor for aqueous SOA. Its reactions with nitrogen containing compounds, both inorganic and organic, have been found to result in the formation of light absorbing aerosols.

Throughout its lifetime, atmospheric aerosols can undergo exposure to different levels of relative humidity (RH). Droplet evaporation at low RH, resulting in a highly concentrated solute environment within the droplet, has been found to accelerate the formation light absorbing compounds. However, studies have shown that the existence of liquid water is highly essential to the production of light absorbing aerosol species, prompting the need for investigating a critical RH level which can effectively facilitate this chemistry.

This study aims to quantitatively describe the effect of RH on the formation of light absorbing aerosols through the reactions of Gly with ammonium sulphate (AS) and Glycine (GL). An initial concentration of 10mM of Gly was mixed with 20mM of AS or 40mM of GL. Each solution was atomized and subsequently dried between 20% and 85% RH. The dried particles were collected on a PTFE filter and extracted with deionised water. Light absorption of aerosol extracts was measured using a UV-vis spectrometer with a liquid waveguide capillary cell. The absorption signals were normalised by the total organic carbon content to obtain the mass absorption coefficient (MAC, m^2/g C) of reaction products observed at different RH levels.

Consistent with previous studies, the Gly-AS system gave a single peak at 287nm while the Gly-GL system gave multiple peaks, with the peak at 380nm being the most prominent. The MAC at the peak wavelengths were plotted against the RH for each system. The MAC of reaction products from the Gly-AS system increased from 100% RH (i.e. bulk solution), reaching a maximum at ∼65% RH. A steady decline of MAC was then observed towards the lower RH. A similar trend was observed for the Gly-GL system with a steady increase of MAC up to ∼55% RH followed by a gradual decline towards the lower RH. Formation of light absorbing aerosol species was insignificant at very low RH condition for both systems. In particular, at ~20% RH, the MAC of reaction products were only comparable to those observed in the bulk solution. Results from both chemical systems highlight the significance of the effect of RH on the production of light absorbing species upon droplet evaporation. The potential influence of phase transition on the formation of light absorbing materials will be discussed.

3AC.4

Marine Organics Alters Sea Spray Physicochemical and Radiative Properties. Aditya Vaishya, JURGITA OVADNEVAITE, Darius Ceburnis, Colin O'Dowd, *National University of Ireland Galway, Ireland*

Nature marine haze layers, predominantly driven by sea spray aerosol, effectively act as mirrors, reflecting back to space part of incoming solar radiation thus modulating global radiation budget. Modulations in the sea spray aerosol physical, chemical, and optical properties on account of enrichment by marine organics may influence the properties, extent, and lifetime of marine haze. Over the North Atlantic waters marine organics constitute significant fraction of the sub micron aerosol population [O'Dowd et al., 2004] during high biological activity (HBA) periods – typically occurring in the months of June, July, and August. Marine air masses, when traversed over the biologically rich North Atlantic waters, bring with them sea spray aerosols enriched with primary marine organics to the coastal measurement station Mace Head (MHD) [O'Connor et al., 2008], on the western periphery of Europe.

We present here the radiative and physicochemical properties of the sea spray aerosols, associated with the low biological activity (LBA) and HBA periods in the North Atlantic, advected to MHD during clean air mass conditions. Aerosol scattering coefficient show a LBA high and HBA low while the spectral scattering exponent shows opposite behaviour. The LBA-high and HBA-low in scattering is found to be driven by contribution of wind-speed generated sea spray aerosols to the marine boundary layer. LBA and HBA scattering values were found be dependent on the square of wind-speed, but LBA scattering values were ~ twice that of HBA scattering values. This apparent difference in LBA-HBA scattering is primarily due to changes in sea spray aerosol chemical composition on account of enrichment by marine organics during HBA periods. Under typical marine boundary layer high humidity fields, sea spray enriched with marine organics are optically less active and their parameterized hygroscopic growth shows a dual state of hygroscopicity flipping from high-hygroscopicity to low-hygroscopicity as the organic volume fraction increases from below ~ 0.55 to above ~ 0.55. The effect of this on Top of Atmosphere (TOA) direct radiative forcing (ΔF) is to reduce the cooling contribution of sea-spray by ~ 5.5 times compared to pure sea-salt spray. Further, using multi-instrument coherent measurement of aerosols properties we show that the LBA-HBA difference in aerosol scattering properties, are not just confined to a change in aerosol chemical composition but also due to change in aerosol dominant size mode, both sub micron and super micron. A shift in dominant aerosol mode to lower sizes, due to organic matter enrichment of sea spray, resulted in increase of aerosol sub micron scattering fraction by over 2.5 times. Combining the effects of changing chemistry and size modes, we show that cooling contribution of sea spray enriched in marine organics is suppressed over 30% under humidity fields associated with cloud base as compare to marine boundary layer humidity fields.

The results presented here highlight a significant coupling between the marine biosphere and the direct radiative budget through alteration of sea-spray chemical composition. The shift to smaller sizes is likely to significant increase the lifetime of the sea spray in the atmosphere, possibly extending the duration and impact of marine haze in the global climate system.

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3AC.5

Impact of Springtime Southeast Asia Biomass Burning on a High-mountain Background Station in East Asia: Aerosol Composition and Light Extinction. SHANTANU KUMAR PANI, Neng-Huei Lin, Chung-Te Lee, Ta-Chih Hsiao, Sheng-Hsiang Wang, *National Central University, Taiwan*

Biomass burning (BB) is well-documented as a significant source of aerosols and trace gases in the atmosphere. Emissions from tropical BB impact the physicochemical and optical properties of the atmosphere. BB affects the Earth-atmosphere energy budget by directly scattering and absorbing the incoming solar radiation and also by indirectly modifying the cloud microphysical properties. BB activities in the form of wildland forest fires and agricultural crop burning are very pronounced over peninsular Southeast Asia (PSEA) mainly in spring (late February to April) season. Springtime regional transport of PSEA BB was investigated over downwind locations in East Asia, for example, the Lulin Atmospheric Background Station, Taiwan (LABS, 23.47°N 120.87°E, 2862 m asl), has been an international well-known site for PSEA BB outflow monitoring. As a part of the Seven South East Asian Studies/Biomass-burning Aerosols & Stratocumulus Environment: Lifecycles & Interactions Experiment (7-SEAS/BASELInE) 2013 campaign, the physical, chemical, and optical properties of aerosols were measured at Doi Ang Khang (DAK, 19.93°N, 99.05°E, 1536 m above sea level, asl), an upwind near-source BB location in northern PSEA, where BB activities were densely distributed in the surroundings. The DAK is an excellent site for investigating the characteristics of near-source fresh BB aerosols and their impacts on regional radiative budget, while the LABS is an ideal site to conduct measurements of long-range transported BB. The objective of the present study is two-fold. Firstly, it investigates the detailed BB signature profiles with reference to water soluble inorganic ions, carbonaceous fractions, monosaccharide anhydrides, and low-molecular-weight dicarboxylic acids in $PM_{2.5}$. Secondly, it estimates the impact and role of aerosol chemical composition on light extinction over both locations. This is the first-time attempt of optical closure study at a high-altitude dynamic aerosol environment. BB aerosols are found more water-soluble in the downwind than the near-source location. Organic matter, ammonium sulfate, and ammonium nitrate are found to be the major contributors to the total light extinction, indicating the dominance of scattering type aerosols than over the absorbing type. This study provides needful information to understand the effect of PSEA long-transported BB on the aerosol composition and radiation budget over a remote and free-tropospheric location in East Asia.

3AC.6

Evidence for Pyrazine-Based Chromophores in Cloudwater Mimics Containing Methylglyoxal and Ammonium Sulfate.

LELIA HAWKINS, Hannah G. Welsh, Matthew V. Alexander, *Harvey Mudd College*

Simulating aqueous brown carbon (aqBrC) formation from small molecule amines and aldehydes in cloud water mimics provides insight into potential humic-like substance (HULIS) contributors and their effect on local and global aerosol radiative forcing. Previous work has shown that these (Maillard type) reactions generate products that are chemically, physically, and optically similar to atmospheric HULIS in many significant ways, including in their complexity. Despite numerous characterization studies, attribution of the intense brown color of many aqBrC systems to specific compounds remains incomplete. In this work, we present evidence of novel pyrazine-based chromophores (PBC) in the product mixture of aqueous solutions containing methylglyoxal and ammonium sulfate. PBC observed here include 2,5-dimethyl pyrazine (DMP) and products of methylglyoxal addition to the pyrazine ring. This finding is significant as the literature of Maillard reactions in food chemistry tightly links the formation of pyrazine (and related compounds) to browning in foods. We investigated both the roles of cloud processing (by bulk evaporation) and pH on absorptivity and product distribution in microliter samples to understand the contribution of these PBC to aqBrC properties. In agreement with previous work, we observed elevated absorptivity across the entire UV/visible spectrum following simulated cloud processing as well as higher absorptivity in more basic samples. Absorptivity of the pH 2 sample, following evaporation, exceeded that of the unevaporated pH 9 sample, indicating that cloud processing can overcome the previously observed kinetic barrier imposed on aqBrC formation in acidic conditions. Further, the fraction of pyrazine compounds in the product mixture increased by up to a factor of four in response to drying with a maximum observed contribution of 16% at pH 5. Therefore, cloud processing under more acidic conditions may produce PBC at the expense of imine and imidazole-derived compounds. This finding has implications for further BrC reactivity and degradation pathways.

3CM.1

Co-benefit of Carbon Dioxide and Air Pollutants Emission Reductions by the Air Pollution Prevention and Control Action Plan in the Beijing-Tianjin-Hebei Region of China. ZHENYU LU, Jun Liu, Mindong Chen, Jianlin Hu, *Nanjing University of Information Science & Technology*

Air pollution problems have become very severe in the Beijing-Tianjin-Hebei region of China due to large amount of air pollutant emissions from intensive fossil fuel consumption. Meanwhile, fossil fuel consumption also emits carbon dioxide (CO2) which is a greenhouse gas and causes climate change. Chinese Central Government has set up the Air Pollution Prevention and Control Action Plan, aiming to reduce air pollutant emissions significant through using cleaner energy, industrial upgrading, eliminating high energy consumption industries, and etc. These actions also have potential in reducing CO2 emissions. In this study, we calculate the synergistic effects of the actions in the plan on main air pollutants and carbon dioxide emissions. The objectives include quantitative analysis of the co-benefit from different industries by different measures for different pollutants in the plan.

The Greenhouse gas-Air Pollution Interaction and Synergies model (GAINS) is used in this study. According to each measures in the action plan, new scenarios with modified activities, energy consumptions, the influence of policy, and the equipment levels are generated in the model. The reductions in the air pollutants and CO2 then are simulated for each of the measures. The results indicate that the potential CO2 emission reduction in Beijing and Tianjin from the measures of reducing coal-fired power consumption is 9.2Mt/year and 4.2Mt/year, respectively. In Hebei, the CO2 emission reduction potential of industrial facilities is the largest, up to 122.5Mt/year. Measures for coal combustion power plants in Beijing contribute the most carbon dioxide emission reduction, accounting for 48% of the total CO2 reduction in Beijing. Measures for industries in Tianjin contributes the largest, reaching 42%. Among the main air pollutants the co-benefit carbon dioxide emission reduction is the highest with NOx in Beijing, is the highest with PM2.5 in Tianjin and Hebei.

3CM.2

Aeolian Dust Deposition and Removal on Surrogate Surfaces with Implications in Solar Energy. Benjamin Figgis, BING GUO, Wasim Javed, Said Ahzi, Yves Rémond, *Texas A&M University at Qatar*

In this study, we measured the rates of dust deposition, rebound and resuspension on surfaces exposed in the dusty desert environment of Doha, Qatar, in order to understand the relation between these rates and the environmental variables airborne dust concentration (PM10), wind speed and relative humidity. An outdoor soiling microscopy (OSM) method was used to acquire images of dust particles on collector surfaces at 10-min intervals over 51 days, from which the rate information was extracted. Meteorological and dust data including wind speed, air temperature/humidity and PM10 were also collected in the same period of time. Air friction velocity was determined using scalar wind speed measurements at two elevations. Various empirical models from previous reports were compared against the present experimental results. It was found that the experimental deposition velocity agreed very well with the prediction of an empirical relation based on the experimentally determined air friction velocity (Kim et al. 2000). However, it was difficult to match the experimentally measured resuspension rate and the available quasi-steady-state empirical relations. This difficulty is presumably because resuspension is not steady-state unless in the hypothetical scenario that the deposited dust is steady-state. This study confirms that dust deposition on solar panels can be modelled adequately using existing models, but a better model is needed to adequately describe dust resuspension from soiled surface.

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3CM.3

Efficacy Assessment of Vegetative Environmental Buffer in Reducing Particulate Matter Emitted from Poultry Houses.

QI YAO, Zijiang Yang, Hong Li, Michael Buser, John Wanjura, Peter Downey, Chen Zhang, Collin Craige, Alba Torrents, Laura McConnell, Gregory Holt, Cathleen Hapeman, *University of Maryland, College Park*

Particulate Matter (PM) emitted from poultry industry have raised concerns due to the potential negative impacts on residents' health and the neighborhood air quality. In the US, Virginia, Maryland, Delaware and Pennsylvania together constructed a developed broiler belt (areas where chickens outnumber people) along the Chesapeake Bay, containing almost 12% of all broilers in the country. This intense broiler farming has led to increased complains about the degrading air quality in the area. Consequently, Vegetative Environmental Buffer (VEB) has been proposed as a cost-efficient, environmental-friendly remediation practice to the poultry industry. Few studies have been conducted to evaluate the actual efficacy of a functioning VEB in reducing PM emitted from commercial poultry houses. In this study, field experiments were conducted to characterize PM, including total suspended particles (TSP), PM_{10}, and $PM_{2.5}$, emission-concentration profiles, as well as to evaluate the effectiveness of VEB in reducing PM concentrations downstream from the poultry houses equipped with VEB. In addition, a modified small-scale Gaussian Plume air dispersion model was used to estimate PM concentration profiles without a VEB under the same meteorological conditions during the sampling period. The results revealed that the diurnal and nocturnal measured PM emission plume shapes were different, which could due to more stable atmosphere at night. VEB promoted the reduction of PM by 20% to 30% based on the comparison between the measured and model-predicted results, which eliminated the diffusion factor.

3CM.4

Development of Hybrid Dust Collector Installed at the In-use Trains for Removing Aerosols in Underground Subway Tunnels. Sang-Hee Woo, SEUNG-BOK LEE, Jong Bum Kim, Jae-In Lee, Gwi-Nam Bae, Moon Se Hwang, Hwa Hyun Yoon, Hong Ryang Jang, Eunserb An, *Korea Institute of Science and Technology*

Airborne particles, or aerosols in underground subway tunnels are mainly composed of metal compounds (Aarnio et al., 2005; Salma et al., 2007; Martins et al., 2016; Moreno et al., 2017), and they have hazardous health risk of passenger and subway workers (Cheng et al., 2012; Park et al., 2014). Therefore, the air quality in the underground subway tunnels should be improved. Generally, a cleaning vehicle or a ventilation system were used to remove dust on the rail ground during traveling or aerosols at the fixed location in underground tunnels, respectively. However, the cleaning vehicle is very slow to clean whole tunnel, and the ventilation system removes particulate matters only in certain areas. In this study, a hybrid dust collector using both an inertial dust collector and an electrostatic precipitator (ESP) in series for application at the in-use subway trains to remove airborne particles from the underground tunnel. Its field performance test was carried out by attaching it to a real subway train.

Two kinds of hybrid dust collectors have been developed. Model 1 has louver as the inertial dust collector for removing large aerosols and one-stage ESP without a fan, and model 2 has baffle and two-stage ESP with a fan. In both cases, EPS was the main component, and inertial dust collector was added to compensate for the disadvantages of the ESP. The each component of the hybrid dust collectors was optimized by wind tunnel experiments. Based on experimental and simulated results, the hybrid dust collectors were optimized to remove the highest weight of aerosols per hour.

After optimizing, the hybrid dust collectors were installed at the in-use train, and operated for 350 hours for 43 days. As a result, the weight of collected aerosols increased linearly with the operating time. Measured weight of collected aerosols was slightly higher than the prediction value based on wind tunnel experiment result, probably because the aerosol concentration at the bottom of the subway train must be higher than that measured at the height of platform. The hybrid dust collector was able to collect 20 to 40 mg of aerosols per 1 km travel distance, and it captured several hundred grams of aerosols during the field test period.

3CM.5

The Effectiveness of Roadside Vegetation Barriers as a Near-Road Air Pollution Mitigation Strategy: A Comprehensive Evaluation of the Sensitivity to Leaf Area Density. KHALED HASHAD, K. Max Zhang, Pradeep S. Prathibha, Jay R. Turner, Daniel Fleischer, *Cornell University*

Exposure to near-road air pollution is a widespread public health concern due to its association with adverse health effects as demonstrated by several epidemiological and toxicological studies. While emission control technologies and programs to directly reduce traffic-related air pollution emissions (referred to as "active" mitigation) are vital components of air quality management, considerable research has been carried out to identify, develop and evaluate "passive" mitigation strategies to reduce exposure to near-road air pollutants (PM2.5, ultrafine particles (UFP), black carbon, NOx and others). Vegetative barriers have been shown to be a promising passive strategy, but their effectiveness depends on leaf area density (LAD) which is often ill-characterized. In our study, we employ three independent methods to estimate the LAD of an engineered vegetative barrier planted in the front lawn of the Saint Margaret Mary (SMM) school in Louisville, KY. The barrier lies parallel to the road and consists of small shrubs, forbs, and trees selected to maximize pollutant removal but not adversely affect dispersion. The three LAD estimation methods include direct sampling of tree branches, optical porosity measurement and voxel-level analysis from ground-based LiDAR remote sensing data. The derived LAD profiles from each method are used as inputs to a high-fidelity computational fluids dynamics model to quantify the reduction of near-road pollutant concentrations for the SMM site, evaluated against observational data including UFP number concentration collected during intensive field measurements. This study marks the first comprehensive assessment of LAD sensitivity. The preliminary results from our study reveal the need to reduce uncertainties associated with LAD estimations and are being used to optimize planting strategies for Green Heart project which is a neighborhood-scale greening study being conducted in Louisville.

3CM.6

Large Scale PM2.5 Cleaning System for Targeted Area with Several Square Kilometers. SHENG-CHIEH CHEN, Min Tang, Qingfeng Cao, David Y. H. Pui, *University of Minnesota*

The Xi'an 60 m (L) x 45 m (W) x 60 m (H) first generation SALSCS has been successfully evaluated and results showed that it can effectively pull urban polluted air containing high $PM_{2.5}$ into the tower by the nature convective flow created by solar irradiation. The high concentration $PM_{2.5}$ was efficiently removed by well-equipped filter bank before the airflow being released back to the ambient. This first generation SALSCS is intended to be scaled up to create a large quanity of clean air to clean up a large urban area. In the second generation SALSCS, the cleaning mechanism of the filtration was modified to raindrop scavenging, a considered green technique. Theoretical calculations have shown that a higher $PM_{2.5}$ removal efficiency could be achieved by reducing the size of water droplets. However, in practical application a reasonable droplet size should be controlled to around 100 to 500 µm for avoiding their reentrainment into the tower. This second generation SALSCS has 20 m x 20 m x 14 m in size and has been built in Salt City of Jiangsu province, China. Experimental evaluation showed that the $PM_{2.5}$ can be collected with >80% efficiency. The $PM_{2.5}$ laden water will be drained into a collecting pond where the water will be processed to remove the $PM_{2.5}$, and the clean water can be recycled and supplied to the sprayers. This will then provide a low cost and sustainable operation for the SALSCS. To be mentioned that the second generation SALSCS is designed to accommodate the use of solar induced convective flow or electrical powered fan as flow driving force. When the nature convective flow is applied, its size also needs to be enlarged. A third generation SALSCS is being developed for a targeted area in densely populated urban area. It has a reduced size but high clean air delivery with the aid of large array of high powered fan. Besides, a special feature of this SALCSC is that the clean air will directly deliver to ground level, a reverse flow direction then the first and second generation SALSCSs. Theoretical calculations showed that a 20 m x 20 m x 20 m third generation SALSCS can produce clean air of ~1000 m^3/s flow rate with 80% $PM_{2.5}$ removal. It is able to clean up an area of 1 km^2 effectively.

3ED.1

Teaching Practical Aerosol Science in the UK. PAUL WILLIAMS, James Allan, Torsten Tritscher, *University of Manchester and NCAS*

Recently in the UK, we have developed a three day course on aerosol science as a partnership between the University of Manchester, The UK National Centre for Atmospheric Science (NCAS) and TSI Europe. While other well-established courses already exist concerning fundamental theory, this course is focused more on application and practical experience for the benefit of scientists coming into aerosol science for the first time, either as part of work or postgraduate study. So far, this course has been run twice with great success and a third course is planned for 2018. The format is a combination of lectures and practical laboratory sessions. The lectures feature guest speakers covering topics such as aerosol properties and mechanics, size definitions and the theoretical basis of various instruments, with a view to providing the foundations of the mathematical techniques and practical skills that an aerosol instrumentation operator would likely use day-to-day. It also covers various applications for aerosol instrumentation, e.g. within industry. Here we will discuss the material covered and the teaching methods utilized. The practical sessions utilized a pool of equipment belonging to the University of Manchester, NCAS and TSI and provided hands-on experience for the operation and maintenance of various instruments (such as DMAs, OPCs, CPCs and aerosol samplers) and also exercises such as characterising losses down different tubing types and dimensions. The course has proved popular with a mix of different attendees, ranging from PhD students and postdocs, technical staff within the academic sector and those from industry.

3ED.2

Hands-On Aerosol Science and Technology Workshops in the Colorado Front Range. SHANTANU JATHAR, John Volckens, Christian L'Orange, Nicholas Good, David Leith, Sherrie Elzey, Aaron Avenido, Tim Johnson, Andrea Tiwari, *Colorado State University*

Colorado State University (CSU) has recently grown its academic and research programs in air quality, climate and human health with 25 faculty and over 50 researchers across 9 departments conducting research in air quality and/or aerosol technology. To supplement aerosol-related coursework offered at CSU and support graduate training in aerosol research at CSU, we organized a series of three-day intensive workshops for researchers in the Front Range of Colorado in the summers of 2015 and 2016 at the CSU Energy Institute. The goal of these workshops was to provide beginners with a hands-on introduction to aerosol measurement while giving seasoned practitioners an opportunity to review the theory and application of aerosol instrumentation. The 2015 workshop was organized around aerosol size and mass measurement and had ~29 participants. The 2016 workshop was organized around personal aerosol exposure measurement and had ~24 participants. Most of the participants at these workshops were graduate students and researchers from CSU although there were a few outside participants from the University of Wyoming, the National Renewable Energy Laboratory, and University of Colorado Denver.

The first two days of each workshop consisted of three sessions. Each three-hour session included a short theory lecture followed by a demonstration or an exercise. Demonstrations were conducted in small groups of eight to ten people and exercises consisted of a small team of three to five people performing an aerosol measurement. In an example exercise from 2015, teams were introduced to filtration-based particle sampling and were later asked to assemble, calibrate, and deploy a filter train to measure particles in an indoor or outdoor environment at the workshop site. An example demonstration from 2016 was one where mid-priced aerosol monitors (e.g., DustTrak, microAeth, UPAS) were setup in different rooms where an instructor, through hands-on interaction, discussed instrument operation and data acquisition. On the final day of each workshop, TSI Inc. organized a full-day workshop that featured their suite of instrumentation to measure aerosols from combustion sources such as diesel engines, cookstoves, and open burning. The TSI workshop included three modules and followed a similar pattern as the first two days: a short theory lecture followed by a demonstration. The demonstrations were interactive where participants were allowed to vary the source type/mode of combustion fuel, actively operate the instrumentation, and change instrument modes/parameters.

Taken together, these workshops introduced students to a wide array of topics within aerosol science and technology: theoretical background, sampling practices, analytical considerations, instrument selection for various applications, instrument operation, and data analysis. Participant counts and engagement in both years suggest that these workshops provide value to the aerosol research community along the Colorado Front Range. Feedback solicited from the 2015 workshop was used to improve elements of the 2016 workshop. Our goal would be to continue to organize this workshop to support aerosol-related activities at CSU and the Front Range in Colorado in the future.

3ED.3

The Earth's Climate and Human Health Taught through the Lens of Clean Cookstoves. DEBORAH GROSS, Tsegaye Nega, *Carleton College*

Air pollution is a leading cause of death globally, with upwards of 4 million deaths per year caused by indoor air pollution due to cooking with biomass fuels, alone (WHO, 2016). This important problem is intimately connected with such issues as combustion and particle emissions from biomass combustion, the environmental impacts due to gathering the fuel, impacts on the global climate from the emissions of soot, and the impact of social structures on the interaction of people, especially women and children, with smoke from cooking fires. To engage fully with this complex problem requires an interdisciplinary approach that forces students and faculty members to stretch beyond standard disciplinary boundaries. This topic, with specific applications to a clean cookstove program in Ethiopia, has been used successfully at Carleton College to introduce undergraduate students to complex climate and health-related issues, while also providing a fruitful topic for faculty teaching and research collaborations. To-date, this project has been connected to 4 classes in three departments on campus, an off-campus program, and the research programs of two faculty members, and we anticipate that its presence will continue to grow. In addition, a class centered around an international collaboration between students at Carleton College and Addis Ababa University, which also includes components of the cookstove study, has been initiated. In this presentation, the centrality of aerosols, and how they can be connected to a range of topics related to climate and health, attracting students from a variety of disciplines, will be discussed.

3ED.4

Introduction to Aerosols Tutorials. RICHARD FLAGAN, *California Institute of Technology*

A set of two Introduction to Aerosols Tutorials has been presented for many years at AAAR. This paper will give a brief overview.

Tutorial 1 is the first of two that introduce the broad field of aerosol science. We begin with the behavior of individual particles to understand how they behave in the environment, and the physical principles on which most aerosol measurements are based. The drag forces that act on a particle determine its settling velocity and whether it is able to follow the flow of a gas. Several different models describe the drag forces: Stokes law applies for spherical particles moving at modest velocities, though a slip correction must be introduced to account for noncontinuum effects for particles small compared to the mean-free-path of the gas molecules. Other corrections are required if the velocity becomes large enough the fluid inertia affects the motion. Knowledge of these scaling principles makes it possible to relate particle behavior in seemingly disparate systems, and make it possible to determine particle size. The drag forces also determine Brownian motion, and, hence, affect their deposition and losses in the respiratory tract, in sampling systems, and in filters, causing aerosol filtration to be more effective than filtration of particles from liquid media. We will briefly look at how this aerodynamic behavior is employed in determining particle size in a wide range of instruments, including the migration of charged particles in mobility analyzers.

Tutorial 2 continues the basic introduction to aerosol science. In this session we focus on developing the tools to describe the dynamics of aerosol populations. An aerosol is an ensemble of particles in a gas, and the particles are distributed over a range of sizes. Therefore, they must be represented by a particle size distribution. We will discuss the representation of aerosol populations as size distributions, their graphical representation, and models such as the log normal-distribution. Condensation and evaporation of volatile species onto particles determines their growth in the atmosphere, and efficient counting of particles too small to detect optically in condensation particle counters. Both continuum and noncontinuum effects must again be considered, as must the surface tension which governs particle activation, initial activation, and the possibility of nucleating new particles from the vapor phase. These processes also alter the shape of the size distribution. Particle-particle collisions lead to coagulation, which further alters the size distribution. We will examine how these diverse processes are combined to describe the population dynamics for aerosol systems.

3ED.5

Air Quality Board Game: A Cooperative Board Game to Play in Class. SAMARA CARBONE, Guilherme Santa Cecília, Lucas Chiari Couver, Frederico Coelho, Jayder Pereira, Amanda Souza, Felipe Roberto Rodrigues, Felipe Jose Carbone, *Federal University of Uberlândia*

In times when information is widely available and often a reason for distraction, creativity is needed to keep the students interest in class. Ludic learning offers an option into that direction restoring the students' motivation and attention. It is in this context that the Air Quality Board Game (AQBG) was created. The AQBG was adapted from Role-Playing Games (RPG) and consists of a cooperative board game, that is, the students play as a team in order to achieve a goal. Typically in RPG, the players roll dice and let them decide on the success of performing a specific action, such as, to open a door, buy an item or attack an opponent. In the AQBG, the players have to answer questions and to solve problems related to the topic in order to succeed in such actions.

The game was designed to be played by teams from three to six players. In this version, the students may choose among the following characters: the city mayor, environmental city counselor, environmental engineer I, environmental engineer II, meteorologist or the Master, each one has specific skills. The background scenery is a medium sized city (500,000 inhabitants) suffering from air quality degradation and the players are this citizen's last hope!

The board was printed in carton paper and is divided into four districts, which are subdivided into 85 moving zones altogether. The districts are industrial, city center, park and residential neighborhood. In the industrial district there are different industries installed, such as, cement, smelter, food factory, paper and cellulose factory, coal power plant, etc. The teacher decides on the type of industries. The players can move between the districts through the moving zones. The districts emit air pollutants, according to its source type, in the pollution turn. There are special tokens spread over the city (shops, university, city hall and hospital) where the players can buy items, receive advices or heal from the adverse health effects of poor air quality.

The game is played in rounds. Each round is composed of three turns. The first turn is the players' turn. Here each player has three free actions. It is considered an action to move between zones, to purchase items, ask for assistance, use/install/replace instrumentation and implement public policies. The second turn is the pollution turn. That is when the pollutants spread over the city. The pollutants move one zone per round, depending on the atmospheric conditions. In the third turn, new pollutants are emitted to the atmosphere by the polluted zones. Cards containing such information decide the pollutant type (PM, CO, NOx, etc) and the emitted amount.

The main goal is to save the city from air quality degradation before the players die from the adverse health effects. Because at every round there are more pollutants emitted by the specific polluted zones, the players must decide on how to act in order to mitigate the air pollution. Each player spends one life when pollutants reach the national air quality reference levels.

One of the ideas under this methodology is to make it as versatile and adaptable as possible. Thus, it could be used in multiple environments. In addition, different items can be included as cards, and the questions could be adapted to different levels of difficulty on the topic.

The AQBG is still under test and some adjustments are still in course. Special items and skills will be added. A preliminary version of the game was well accepted by the students enrolled in the Air Pollution Control coarse. The students will answer a questionnaire to expose their opinions about playing the game.

3ED.6

McDonnell Academy Energy and Environment Partnership (MAGEEP) Education Network: MAG^{E}Net. BEDIA KARAKOCAK, Tandeep Chadha, Jeff Yang, Orhan Yenigun, Prasad Modak, Pratim Biswas, *Washington University in St Louis*

As a part of McDonnell Academy Energy and Environment Partnership (MAGEEP), McDonnell Academy partner universities are networked and collaborating on various projects related to energy and environment. The consortium of 35 universities and corporate partners work together on energy, environmental, and sustainability research, education, and operations. MAGEEP's mission is to collectively identify and collaboratively tackle important global energy and environmental challenges in an integrated and holistic manner. In addition to the university partnerships, to unite all 35 MAGEEP partners with industry and non-governmental organizations on education, MAGEEP Education Network (MAG^{E}Net) was established in 2015. Each partner university has its own training and degree programs in energy and environment-related areas. The MAG^{E}Net is, however, based on co-utilizing the educational resources and expertise of all faculty at the 35 institutions. An added advantage is in the networking with the corporate sector and developing a model for education with links to industry, government, and non-governmental organizations. An exclusive framework is proposed as a networked approach to establish courses and certificate programs on energy and environment while developing a model for education with links to industry, government, and non-governmental organizations. The overall network will be guided by a MAGEEP educational advisory committee consisting of faculty members from interested institutions. We will demonstrate the use of a CANVAS platform to illustrate how educational modules are set up. Specifically, we will give examples of aerosol modules that have been set up on this platform.

3IA.1

Evaluation of Mobile Air Purifiers under Realistic Conditions. STEFAN SCHUMACHER, Daniel Spiegelhoff, Miriam Küpper, Ute Schneiderwind, Hartmut Finger, Christof Asbach, *Institut für Energie- und Umwelttechnik e.V. (IUTA)*

Over the last years, air pollution has more and more moved into the focus of public attention. This not only concerns the atmospheric pollution, but also the indoor air quality, which can be deteriorated either by infiltration from outside or by indoor sources. Since people in industrial nations spend most of their time inside buildings, the latter is of special importance. A way to improve the indoor air quality are mobile air purifiers, which draw the polluted air through a filter (here a fibrous electret filter) and release the purified air back to the room so that the pollutant concentration decreases exponentially with time.

Different national standards classify the cleaning performance of mobile air purifiers by their clean air delivery rate (CADR), which describes the flow rate of clean air delivered by the air purifier. It is determined by measuring the temporal decay rate of an initial pollution concentration in a closed room while the air purifier is running. Most standards only consider the number concentration of particles larger than 0.3 µm, although relevant indoor aerosols mainly consist of much smaller particles. To address the question whether such CADR measurements yield a praxis-oriented measure, the size-dependent CADR for particles down to 0.03 µm was investigated. It was found that the CADR significantly drops with decreasing particle size, which means that recent standards overestimate the cleaning efficiency with respect to many relevant indoor aerosols.

It is known that the efficiency of electret filters can drastically degrade with time due to exposure to particles, gases, or humidity. Therefore, we developed a method to reproducibly age the filters by burning cigarettes in steps of 12 at the same time in a 25 m^3-room (Finger 2015). Also the aging behaviour strongly depends on the particle size, which can be explained by the size dependence of the electrostatic contribution to the total filtration efficiency (Schumacher 2018). Furthermore, the results were compared to aging with 48 cigarettes at the same time in a 3 m^3-cube as proposed by a recent Chinese standard, which yields a very distinct aging behaviour. This shows that for a praxis-oriented rating of the long-term stability the considered particle size range and the conditions of aging are of great importance.

Standardized tests are always conducted in test chambers without furnishings and with good air mixing. In contrast, in occupied rooms the flow and hence the pollutant dispersion can be much more complex. To investigate possible deviations, an air purifier was operated in an office room with the pristine outdoor aerosol as target pollutant. To measure the local CADR, portable particle monitors based on diffusion charging were located at different positions in the room. At all tested positions they showed similar decay curves, indicating that the cleaned air was homogenously distributed within the room. Also the location of the air purifier did not have a significant influence. However, the CADR determined in the office room was generally slightly smaller than in the standardized test chamber, which might be attributed to the different particle size distribution of the test aerosols.

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3IA.2

Measurement of the Fractional Deposition Efficiency of Full Scale HVAC and HEPA Filters for Nanoparticles ≥ 4 nm.

CHRISTOF ASBACH, Tobias Schuldt, Frank Schmidt, Wolfgang Mölter-Siemens, Ana Maria Todea, *IUTA, Duisburg, Germany*

Concerns regarding adverse effects of nanoparticles, e.g. concerning human health upon inhalation, or product quality upon deposition on clean production equipment or the eventual product, such as semiconductor chips, have increasingly been raised over the recent years. Consequently, these particles have to be removed from the supply air for e. g. residential or office buildings or cleanrooms. It is well known from filtration theory that such small particles are efficiently captured in filters because of their high diffusivity. Methods for determining the fractional deposition efficiency are only available and well established for filter media, whereas no such method has existed up to now for full scale HVAC filters. This is mainly due to the lack of suitable particle generators that provide such small particles in sufficient concentrations to test the filters at flow rates of up to several thousand cubic meters per hour. The high efficiency of filters for nanoparticles necessitates very high upstream concentrations in order to still be able to measure the downstream particle size distribution. If the particles are (quasi-) monodisperse, then it would also suffice to only measure the total particle concentration downstream, which can be done even for very low concentrations.

In the present work, we used a flame based nanoparticle generator (FG2, MoTec Konzepte, Bochum, Germany), in which a sodium chloride solution is continuously fed into a hydrogen-oxygen flame, where it evaporates. Upon cooling, the sodium chloride vapor nucleates to produce very small particles at very high concentrations. The so-produced aerosol is mixed with the filtered air in a test rig according to EN 779/ISO 16890 (also comparable to ASHRAE 52.2), in which the test filter is installed. The modal particle diameter can be adjusted between approximately 4 nm and 70 nm via the sodium chloride concentration in the solution, the feed rate of the solution, as well as the residence time of the freshly produced aerosol in the injection system before it mixes with the high flow rate. The generated aerosols are quasi-monodisperse (according to VDI 3491-1) with geometric standard deviations mostly between 1.3 and 1.5 and particle concentrations upstream of the filter in the range of 1e6 1/cm^3 to 1e7 1/cm^3. To extend the tested size range up to 100 nm or to increase the monodispersity of the evaluated NaCl particles, the aerosol particles in the flow sampled from the test rig can be classified with a differential mobility analyzer (DMA) at a fixed voltage. If information on the collection efficiency for particles >100 nm is desired, a DEHS test aerosol can be used. A correction procedure to account for multiply charged particles upon classification with a DMA has been developed and successfully tested. Several new and artificially aged filters ranging from F7 (according to EN 779, comparable with MERV 13 according to ASHRAE 52.2) to H13 (according to EN 1822) have been tested using the newly developed method and set up. The results typically compare well with those obtained from media samples. The experimental set up and test procedure will be presented along with the data from the filter evaluations.

3IA.3

Quantitative Filter Forensics to Assess Indoor Exposures. Raheleh Givehchi, Juan Pedro Maestre, Chenyang Bi, Kerry Kinney, Ying Xu, Dennis Wylie, Sharon Horner, JEFFREY SIEGEL, *University of Toronto*

The aim of this study is to assess the integrated average indoor airborne concentrations of particle-bound contaminants from dust extracted from heating, ventilation, and air conditioning (HVAC) filters by employing a novel quantitative filter forensics (QFF) approach. QFF allows for the estimate of integrated airborne concentrations of concentrations over the duration that the filter was installed and thus has potential to be a useful method to assess indoor airborne exposures. We extracted the dust from HVAC filters in 60 homes located in central Texas, USA. Filters were collected after one month of deployment in both summer and winter. Dust recovered from these filters were characterized for particle-bound contaminants including total fungal and bacterial DNA (using qPCR with generic primers), 36 common fungi species (with qPCR and species-specific primers), endotoxins, and semi-volatile organic compounds (SVOCs). When combined with HVAC system characterizations including system runtime, air flow rate, and filtration efficiency, we calculated the average airborne concentrations of each analyte in the homes in both seasons. The results showed considerable differences between the concentrations of airborne particle-bound contaminants between homes and it is not clear if short-term tests would capture these differences. In general, no statistical differences were observed for concentrations of contaminants between winter and summer. In this sample of homes, the HVAC measurements varied much less between homes than the dust concentration measurements, suggesting that even in the absence of HVAC data analyzing the dust on filters can provide insight about exposures about a relatively homogenous group of buildings. This study confirms the feasibility of the QFF approach to estimate airborne concentrations for a variety of particle-bound contaminants.

3IA.4

Application of the Time-of-Wetness Model to Fungal Growth in Carpet Dust. SARAH HAINES, Karen C. Dannemiller, *Ohio State University*

Microbes in carpet dust represent a major source of human exposure due to resuspension from occupant motion. Our previous work has established that elevated relative humidity in the air is sufficient to support microbial growth in dust. However, typical diurnal variations occur in buildings and it is poorly understood how this may affect growth. The goal of this work was to apply the time-of-wetness model from fungal growth on drywall to model fungal growth in carpet dust. We collected used carpet and dust from 12 homes. We inoculated 10 x 10 cm carpet coupons with dust from the same home and incubated it at 50% equilibrium relative humidity (ERH) and then raised it to either 85% ERH or 100% for 0, 6, 12, 18, or 24 hours per day. Relative growth rates were then calculated using fungal concentration measured by quantitative Polymerase Chain Reaction (qPCR). Results were consistent with the time-of-wetness model, and may have demonstrated activation limited growth. Pearson correlation coefficients for 85% ERH was c 0.898 and for 100% ERH was 0.958. Dominant taxa at elevated ERH were Aspergillus and Penicillium species, among others. Overall, we demonstrate that the time-of-wetness model can be used to model fungal growth in carpet dust.

3IA.5

Measuring Size-Resolved Indoor Particle Concentrations in Single-Family Homes with Asthmatic Residents: A Chicago Field Study. PARHAM AZIMI, Brent Stephens, *Illinois Institute of Technology*

Human exposure to a variety of airborne pollutants such as particulate matter is often greater indoors than outdoors, particularly in residences where people spend most of their time. In fact, indoor exposure to PM2.5 in residences is estimated to account for the vast majority of the chronic disease burden associated with residential indoor air pollution. Moreover, one study recently estimated that residential exposures account for approximately 40% of the childhood and adult asthma prevalence in the U.S., where nearly 8% of the population has been diagnosed with asthma. However, few studies have elucidated the long-term contributions of indoor and outdoor sources to indoor PM concentrations in residences with asthmatic residents. Therefore, the goal of this study is to measure the size-resolved indoor and outdoor concentrations of particles (0.3 to 10 µm using an optical particle counter) in addition to several other pollutants in 45 single-family homes with asthmatic residents in Chicago, IL over a yearlong period. Each home is visited four times per year, with approximately weeklong monitoring periods occurring once per season. Simultaneous measurements of indoor and outdoor particle concentrations will allow for estimating the relative contribution of indoor and outdoor sources by estimating infiltration factors using a censoring algorithm. This work is also part of a larger study to investigate the effectiveness of three common approaches to upgrading residential mechanical ventilation systems in existing homes for reducing indoor pollutants of both indoor and outdoor origin and improving asthma-related health outcomes. These results will be treated as the background measurements before upgrading the mechanical ventilation systems of the participants' homes.

3IA.6

Estimates of Fine and Ultrafine Particle Removal Efficiency for Residential HVAC Filters Using In-Situ Size-Resolved Efficiency Measurements. TORKAN FAZLI, Brent Stephens, *Illinois Institute of Technology*

Central HVAC filters are commonly evaluated for their size-resolved particle removal efficiency by challenging them with a test aerosol in a laboratory setting. However, aerosol classifications that are most commonly used in regulatory monitoring and building measurements typically include integral measures of mass-based concentrations or total number concentrations. Because filter test standards have not traditionally considered these measures, building owners, occupants, and other key personnel cannot make informed decisions on HVAC filtration for these measures. Moreover, because the removal efficiency for integral measures of $PM_{2.5}$ and UFP are also a function of particle size distributions that challenge the filter, one has to consider the varied sources of aerosols found indoors and their size distributions. This work has two objectives: (1) to measure the in-situ size-resolved particle removal efficiency of off-the-shelf residential HVAC filters, and (2) to use these size-resolved efficiency data to estimate integral measures of $PM_{2.5}$ and total UFP removal efficiency for the same filters for typical residential indoor settings based on a survey of indoor particle size distributions. Particle concentration measurements were made upstream and downstream of a wide range of commercial available filters with various minimum efficiency rating values installed in a central air handling unit in an unoccupied residential apartment unit. Next, a literature review was conducted to gather a variety of indoor particle size distributions (PSDs) from across the world and tri-modal lognormal distributions were fit to each of them. Finally, the particle removal efficiency for each filter for integral measures of indoor UFPs and $PM_{2.5}$ were calculated for each indoor PSD. In-situ size-resolved measurements indicate that filters with similar rating values but from different manufacturers can have very different removal efficiencies for $PM_{2.5}$ and total UFPs, and that the assumption for indoor PSDs can greatly impact estimates of removal efficiency.

3IN.1: INVITED

The Role of Ice Nucleating Particles in Convective Aggregation. HASSAN BEYDOUN, Corinna Hoose, *Karlsruhe Institute of Technology*

Deep convection is the primary mechanism by which energy is vertically transported in the tropical atmosphere. This energy transfer, manifested through latent heating by clouds, counteracts top of the atmosphere radiative cooling. Radiative-convective equilibrium (RCE) is a state in which these two modes of energy transfer balance, and has been shown to be a good approximation of the tropical atmosphere.

For over two decades now, numerical simulations of radiative-convective equilibrium at the cloud resolving scale have unraveled a phenomenon termed convective aggregation, whereby deep convection clusters into a single region of the domain. The implication is a polarized atmosphere, in which one region is dry and clear while the other is cloudy and rainy. Cloud ice is a key element in RCE due to the latent heat release of freezing, the radiative warming induced by anvil and cirrus clouds, and ice's role in precipitation formation. Despite ice's contribution to all key modes of the atmosphere's energy exchange within itself and with its boundaries, no study has yet quantified the sensitivity of the RCE state to ice microphysics and subsequently the sensitivity to aerosol perturbations through ice nucleating particles.

We conducted RCE simulations with the ICOsahedral Non-hydrostatic atmosphere large eddy model (ICON-LEM) on a 700km x 700 km domain with periodic boundary conditions, a two moment microphysics scheme, and a fully interactive radiation scheme. Changes made in each simulation were the ice nucleating particle (INP) concentration, the inclusion (or omission) of the secondary ice formation by the Hallet-Mossop mechanism, and the temperature onset for homogenous freezing. Higher INP concentrations exhibited two fingerprints on the microphysical structure: decreased high altitude ice clouds and increased surface precipitation. Both these effects stem from the lower height at which liquid is converted to ice in the high INP configurations. We found a consistent trend in the simulations' effect on the RCE state, whereby configurations which enhanced precipitation led to stronger convective aggregation. This is tied to the increased latent heat flux at the surface and decreased high level cirrus clouds which act to reduce the longwave cooling in the dry regions of the domain. However, the magnitude of these effects is very sensitive to the other ice formation processes of homogenous freezing and secondary ice formation. Increasing (or decreasing) the onset temperature of homogenous freezing can dampen (or amplify) the sensitivity to INPs active at low temperatures while inclusion of the secondary ice formation process has a similar impact of INPs active at high temperatures. The implications of these results on mixed phase clouds, deep convection, and climate will be discussed.

3IN.2

Molecular Perspective on Water Vapor Deposition onto Ice Surfaces. Daniel Schlesinger, Samuel J. Lowe, Xiangrui Kong, TINJA OLENIUS, Jan B. C. Pettersson, Ilona Riipinen, *Stockholm University*

Condensation of water molecules from the vapor phase onto liquid water and ice surfaces plays a crucial role in atmospheric processes. In the present study we focus on the accommodation of water molecules from the vapor phase into the bulk crystalline ice phase. Experimental data suggest that the bulk accommodation coefficient decreases with increasing temperature but data from different experiments are spread over a large range of values indicating large uncertainties (Kong et al., 2014; Skrotzki et al., 2013). The results presented here are obtained combining a refined analysis of recent experimental data with molecular dynamics (MD) simulations. MD simulations are specifically used to investigate the role of the disordered interface of ice in depositional growth processes of the crystal phase.

3IN.3

Sensitivity of Ice Cloud Formation and Precipitation Initiation to Global Distribution and Abundance of Ice Nucleating Particles in E3SM. KAI ZHANG, Xiaohong Liu, Hui Wan, *Pacific Northwest National Laboratory*

Ice nucleating particles (INP) in the atmosphere affect ice cloud formation and can potentially initiate precipitation. However, ice cloud often doesn't appear near regions with largest INP concentrations, because the distribution of supersaturation (that is dependent on water vapor and temperature) and temperature are also important factors. In this study, we evaluated the global distribution and abundance of INP in the Energy Exascale Earth System Model (E3SM) and identified several important regions based on the co-occurrence of INP, supersaturation, and low temperature. We performed simulations with perturbed INP concentrations and investigated the competition between different ice nucleation mechanisms. Impact of spatial variability in vertical velocity and water vapor inside the GCM-grid on ice nucleation is represented in the model using the predicted statistical distribution of updraft velocity and water vapor. Results show the perturbed INP concentrations have various impact on ice cloud formation and precipitation initiation in different regions. The impact on cloud radiative forcing will also be discussed.

3IN.4

Evaluation of Immersion Freezing Properties of Dark-Colored Particles under Mixed-Phase Cloud Conditions. YUTAKA TOBO, Nobuhiro Moteki, Kouji Adachi, Sho Ohata, Atsushi Yoshida, Makoto Koike, Yutaka Kondo, *National Institute of Polar Research*

Dark-colored aerosols are thought to have an influence on the Earth's climate system by heating the atmosphere and by reducing snow albedo. It is well recognized that black carbon (BC) is a major type of dark-colored particles. In addition, recent work has shown that certain amounts of anthropogenic iron oxides having similar color and morphology to BC are present in the atmosphere. Understanding the influence of such dark-colored aerosols on heterogeneous ice nucleation is important to evaluate their impact on ice formation in supercooled clouds and subsequent ice-induced precipitation (i.e., their deposition process to the snow surface); however, their ice nucleating ability remains uncertain and controversial. In this study, we evaluate the roles of different types of dark-colored particles (e.g., BC, iron oxide) as ice nucleating particles (INPs) under conditions relevant to mixed-phase clouds. Immersion freezing experiments using an original cold-stage-based technique (NIPR-CRAFT) indicate that although the particles used here can serve as INPs at temperatures colder than -20°C, their ice nucleating abilities are much lower than those of other types of insoluble particles reported previously. Furthermore, based on field measurements and modeling estimates, we suggest that the contribution of the dark-colored particles to the population of INPs in the atmosphere may be negligibly small, at least in the Arctic region.

3IN.5

The Development and Characterization of a “Store and Create” Microfluidic Device to Study Ice Nucleation Particles.

THOMAS BRUBAKER, Michael Polen, Leif Jahn, Perry Cheng, Vinay Ekambaram, Shelley Anna, Ryan Sullivan, *Carnegie Mellon University*

Characterization of heterogeneous ice nucleation by ice nucleating particles (INPs) is hindered by the analytical challenge of accurately determining the freezing temperature spectrum and atmospheric concentration of these rare one-in-a-million ice nucleating particles (INPs). We have developed a microfluidic device interfaced with our cold plate system with a greatly improved background homogeneous freezing background signal from pure water droplets compared to droplets on a substrate methods. The lower consistent background freezing temperature spectrum enables measurements of weaker but often more abundant INPs that induce freezing near -30 °C, such as found in biomass burning aerosol. We used soft lithography techniques to fabricate our microfluidic device from PDMS. A “store and create” method is used to form and trap an array of uniformly sized droplets. The aqueous droplets have minimal surface interactions with the rigid device since the surfactant-less oil preferentially coats the hydrophobic walls, ensuring the droplets do not contact the polymer surface. Our homogeneous background freezing signal has a median freezing temperature of T_{50}=-33.88± 0.46 °C. The freezing of the droplets was imaged on a gold-plated silicon wafer using reflectance microscopy. An automated script analyzes the images producing the frozen fraction curves and size distribution of our droplets. We characterized our system using SnoMax, illite, Arizona test dust particles, pure water, aged and fresh biomass burning aerosol, and commercially available 100 nm metal oxide nanoparticles. The metal oxide nanoparticle’s near-monodispersed surface properties enable us to begin decoupling different ice nucleation pathways and study INP behavior in a systematic fashion.

3IN.6

Enhancement of the Heterogeneous Ice Nucleation by the Phase State Change of Organic Aerosols. YUE ZHANG, Martin Wolf, Leonid Nichman, Zhenfa Zhang, Avram Gold, John Jayne, Paul Davidovits, Douglas Worsnop, Jason Surratt, Timothy Onasch, Daniel Cziczo, *MIT; Aerodyne Research, Inc.; UNC Chapel Hill*

Cirrus clouds and their effects on earth's radiative balance are major sources of uncertainties in predicting future climate. These clouds also dehydrate air ascending to the tropopause, thereby reducing water content in the stratosphere. However, the formation of cirrus clouds is not well understood. Data from field sites and campaigns have shown that organic aerosols (OAs) dominate the non-refractory aerosols in the free troposphere where ice cirrus clouds typically form. Measurements by aerosol mass spectrometers over forests indicate a high mass fraction of these OAs are derived from the atmospheric oxidation of isoprene and other volatile organic compounds (VOCs). Despite their abundance, the effects of these OAs on ice nucleation (IN) is controversial. Previously, these OAs were assumed to be homogeneously mixed liquids, which limits their IN properties. Recent studies have shown that depending on the ambient humidity and temperature, OAs can exist in semi-solid or solid phase states, which can potentially increase IN activity. This laboratory study systematically examines the effects of aerosol-phase state on IN properties of OAs by using the spectrometer for ice nucleation (SPIN), a commercially available instrument manufactured by Droplet Measurement Technologies, Inc.

Organic aerosols comprised of representative surrogates and the actual components of isoprene photo-oxidation products were generated and passed through a temperature control apparatus, where the temperature of the aerosols can be varied between -25°C and 13°C before entering the SPIN. A scanning mobility particle sizer (SMPS) measured the number-diameter distribution of the particles upstream of the SPIN. An optical particle counter downstream of the SPIN measured the optical signatures of the ice particles and some of the large bare organic particles. The SPIN operating temperature was between -38°C and -46°C. Our results show that pre-cooling the aerosol particles to -25°C enhances the IN onset relative humidity (RH) and the active fraction of IN when compared with non-pre-cooling conditions. Coupled with viscosity and glass transition temperature calculations, we show that the aerosol phase state changes due to the pre-cooling is the reason for this enhancement.

2-Methyltetrol, a multiphase reaction product in the isoprene secondary organic aerosol (SOA) that exist in ambient aerosols, was aerosolized, temperature controlled, and measured by the SPIN. The glass transition temperature of 2-methyltetrol as a function of relative humidity was parametrized based on measurements from dielectric relaxation spectroscopy. Results show that as the viscosity of 2-methyltetrol increases, the IN onset relative humidity decreases (i.e., IN activity increases).

Our study suggests that the phase state of organic aerosols, governed by their chemical composition, affects their IN properties. As the phase state of the organic aerosols changes from liquid to semi-solid or solid, their IN onset relative humidity decreases, sometimes by 10% RH. The isoprene SOA product molecule used in this study suggests isoprene SOAs may be important ice nuclei in the free troposphere.

3MD.1

Improving Single Particle Aerosol Mass Spectrometry (SPAMS) Inhalation Analytics Performance through Rapid Particle Tracking and Sizing. Martin Jetzer, Bradley Morrical, DAVID FERGENSON, Georgios Imanidis, *Novartis Pharma AG*

The two primary challenges in the analysis of inhalational pharmaceuticals and their associated devices (inhalation analytics) are the determination of the aerodynamic particle size distribution (APSD) of the active pharmaceutical ingredients (APIs) and, in the case of combination products, their co-association at the level of the individual aerosol particles. Additional challenges include formulation optimization (via excipient addition or process alteration) and the analysis of device and formulation performance under varying physiological conditions. A unique requirement for any inhalation analytical method is that it must handle a very large load of particles over a very short period of time. Multiple APIs in different combinations and the presence of non-API carrier particles require the composition of individual aerosol particles to be determined, rendering conventional particle counter/sizers substantially ineffective. The preferred method for determining the APSD of orally inhaled pharmaceutical aerosols according to the compendial literature is cascade impaction (for example the Next Generation Impactor, NGI, Copley Scientific, UK) followed by high performance liquid chromatography (HPLC). While highly quantitative for the total concentration of API delivered, this technique does not yield any information regarding the co-associations between the various product components (APIs and excipients) within the formulation. Single Particle Aerosol Mass Spectrometry (SPAMS) was initially applied to inhalation analytics to address this issue.

A SPAMS instrument collects a dual polarity mass spectrum from up to 250 individual particles per second and records the aerodynamic diameter of each particle as well. Unlike predecessor instruments, which froze or returned nonsensical data under heavy particle loads, a SPAMS continues to acquire up to 250 randomly sampled aerosol mass spectra per second under essentially arbitrary aerosol conditions. Because a SPAMS uses a single, square tracking laser that is roughly 1 mm tall, even under very high particle concentrations only a single particle will typically be in the tracking region at a time. The light scatter trace is acquired over a period of ~100 microseconds for each particle so it is also possible to verify that the particle was alone in the mass spectrometer.

However, until now there was no way to estimate the degree of particle load saturation occurring in a SPAMS measurement. Lacking this information, it was necessary to parametrically calibrate SPAMS data versus an NGI/HPLC analysis or a conventional counter/sizer such as a TSI 3321 Aerodynamic Particle Sizer. We have now developed a firmware upgrade to SPAMS, Survey Mode, specifically for inhalation analytics, which is similar to Fast Scatter Mode on the TSI Aerosol Time-of-Flight Mass Spectrometer but with significant additional capabilities. In Survey Mode, a SPAMS observes all aerosol scattering events that occur within the tracking laser over a full second. This allows the SPAMS not only to determine the absolute numbers and the sizes of the particles entering the instrument but also to determine the fraction of the time that any particles are found within the tracking laser, ensuring the integrity of the mass spectra that are acquired in the surrounding times.

We report the analyses of several combination inhalational pharmaceutical products in alternating Survey and mass spectrometric acquisition modes. We observe the progress of the SPAMS from saturation to non-saturation conditions and scale the mass spectrometric data to the total observed aerosol. Simultaneous measurements were made using a TSI 3321 APS to verify the linearity of the SPAMS survey mode. Scaling factors were determined for the SPAMS data, which are expected to be durable across many different aerosol systems.

3MD.2

Directly Measuring the Rapid Evaporation/Growth of Metered Dose Inhaler/Dry Powder Inhaler/Nebulizer Formulations. ALLEN E. HADDRELL, David Lewis, Tanya Church, Jonathan P. Reid, *University of Bristol*

Targeted delivery of pharmaceuticals in the lung could result in less required total dose, lowering exposure time, prevalence of side effects and overall cost. A consensus forum of industrial, academic and regulatory experts identified a poor understanding of the relationships between physicochemical characteristics of drug formulations and performance in the humid environment of the respiratory tract as one key barrier to progress in inhalation therapeutics (a). Thus, quantifying the properties of pharmaceutical aerosol that govern hygroscopic growth will yield the potential for the rational design of new formulations for drug delivery to the lung. The ability to control the hygroscopic growth of inhaled pharmaceutical aerosol to improve drug efficacy through targeted dosing has received renewed interest in recent years.

Broadly speaking, the delivery of an active pharmaceutical ingredient (API) from a starting formulation to the deep lung involves three phases: aerosol generation, transport from the aerosolization device to the mouth, and concludes with inhalation/deposition. The deposition rate in the lung is controlled by the aerodynamic diameter of the droplet at the time of deposition. Thus, the size of the droplet at the point of generation, the reduction in droplet size resulting from the net loss of volatile mass (if present) during transfer from the device to the mouth, and any hygroscopic growth on inhalation will have a dramatic effect on total and regional dose. The interplay between these complex processes are explored here.

The novel aerosol analysis technique for measuring the hygroscopic properties of surrogates of ambient aerosol, the comparative kinetic electrodynamic balance (CK-EDB) was used in this study. Capabilities that are unique/advantageous to the CK-EDB include:

(1) Use of a water droplet to probe the RH of the airflow that the sample droplet is subsequently studied in with accuracy of ±0.1%, an order of magnitude better than conventional RH probes.

(2) Direct measurement of the dynamic behaviour of a droplet of known composition in a static and/or variable environment (resolutions of 50 nm and <100 milliseconds).

(3) Accurate determinations of the radial growth factor, a measure of the equilibrium hygroscopic growth of the aerosol as a function of gas phase RH across a range of RH from dry to >99%, and with temperature ranging from <50C to <-30C. samples.

To be presented are the kinetic and thermodynamic hygroscopic properties of commercially available nebulizer, DPI, and MDI formulations as measured by the CK-EDB.

(a) Forbes, B. et al., Adv. Drug Del. Rev. 2010, 63, 69–87.

3MD.3

Biokinetics of Aerosolized Liposomal Ciclosporin a in Human Lung Cells in Vitro Using an Air-Liquid Cell Exposure System (Alice). OTMAR SCHMID, Corinne Jud, Yuki Umehara, Dominik Mueller, Albert Bucholski, Friedrich Gruber, Oliver Denk, Roman Egle, Alke Petri-Fink, Barbara Rothen-Rutishauser, *Helmholtz Zentrum Munchen, Comprehensive Pneumology Center*

Background

Inhalation of drugs in aerosolized form is a promising route for non-invasive targeted drug delivery to the lung. Nanocarrier systems such as liposomes have been explored for inhalation therapy opening new avenues including stabilization of non-soluble drugs (e.g. Ciclosporin A (CsA)) and controlled release. Optimized aerosol delivery technologies are required for implementing aerosols into the early preclinical phases of drug testing (instead of pipetting of substances).

Methods

The previously introduced ALICE (Air-Liquid Interface Cell Exposure) system equipped with an investigational eFlow® Technology vibrating membrane nebulizer has been used for an in vitro study of the biokinetic behavior of nano-sized liposomes loaded with the immunosuppressive drug CsA (L-CsA) at the lung epithelial barrier. Human lung epithelial cells (alveolar A549 and bronchial 16HBE14o- epithelial cells) were exposed to aerosolized L-CsA at the air-liquid interface (ALI) and the temporal profile of the L-CsA dose in the apical, basal and cell compartment were monitored up to 24h.

Results

Aerosolization of different volumes of L-CsA solution with the ALICE resulted in dose-controlled, efficient (ca. 7% of invested substance reached the cells), spatially uniform (<8% SD for different inserts) and reproducible L-CsA (<12% SD) delivery. The measurements were performed under non-toxic conditions as determined by cell viability in pro-inflammatory cellular response at 24h post-exposure. The biokinetics analysis revealed that both cell types formed a tight but imperfect barrier for L-CsA resulting in initially high transbarrier L-CsA transport rates, which ceased after about 4h. This burst-like L-CsA transport profile, which is typically also observed in patients, cannot be observed with standard non-aerosolized (submerged) biokinetics assays. Moreover, a 150-fold higher L-CsA concentration was established in the apical (air-exposed side of the cells) and cell compartment compared to the basal compartment (“blood” exposure side of cells). Most importantly for pulmonary drug targeting, a high cellular L-CsA dose level (20-25% of the delivered dose) was obtained rapidly (<1h) and maintained for at least 24h suggesting rapidly established and uniform drug levels in the lung epithelium.

Conclusions

The ALICE exposure system combined with lung epithelial cells cultured at the ALI offers a reliable and relevant in vitro platform technology to study the effects of inhalable substances such as L-CsA under biomimetic conditions.

3MD.4

Formulation Development and In Vivo Pharmacokinetics of Topotecan for Targeted Treatment of Lung Cancer. PHILIP KUEHL, Michael Burke, Ramesh Chand, Devon Dubose, June Liu, Mathewos Tessema, *Lovelace Biomedical, 2425 Ridgecrest Dr. SE, Albuquerque, NM*

Purpose: Lung cancer remains one of the leading causes of cancer death worldwide with approximately 10% to 15% of lung cancers are of small cell histology. Small cell lung cancer (SCLC) has a very aggressive course, with a median overall survival of about 1 to 2 years with only up to 12% of patients surviving for 5 years after diagnosis even in early stages of the disease. Topotecan (TPT) is a FDA approved chemotherapeutic agent that is active in the treatment of SCLC and is one of the only second-line treatment options. TPT is currently delivered by oral or IV delivery and some patients encounter adverse side effects. Therefore, a novel spray dried powder formulation of TPT has been engineered for inhalation delivery to allow for the direct delivery of this potent compound in a non-obtrusive way and limit systemic exposure. This developed formulation was evaluated in non-clinical rodent pharmacokinetic studies to quantify local drug concentrations at the site of action. The local drug concentrations at the site of action will be used to select dose(s) for non-clinical efficacy models.

Methods: A powder fit for pulmonary delivery through inhalation containing TPT free base was developed and spray-dried on a small-scale custom spray dryer (BLD-35) with 35kg/hr. drying gas capacity from a 100% aqueous solution at 4wt% solids. The solution was adjusted to a pH of 3.5 using HCl to ensure complete dissolution of TPT. Functional excipients, Trehalose and L-leucine, were added for additional stability and particle formation. The developed formulation was characterized for solid state, chemical and aerosol characteristics to confirm its formulation applicability. The formulation was evaluated in a rat nose-only inhalation exposure pharmacokinetic study. The IV dose was 0.7 mg/Kg based on the scaled clinical dose and two inhalation doses of 0.14 and 0.79 mg/kg were delivered. Aerosols were monitored for total aerosol concentration, topotecan aerosol concentration and particle size distribution. Following dosing animals were serially sacrificed for systemic blood and plasma analysis by LCMS. Average concentration versus time profile modeled with non-compartmental analysis.

Results: The final dry powder was 70/20/10 Trehalose/Leucine/TPT (w/w%) and was characterized to be highly respirable free from fusion. The final formulation contained amorphous Trehalose and TPT while also having crystallized leucine character. Testing in a clinical device indicated emitted fractions from a capsule and device was 94.0 ± 3.3 % and the corresponding MMAD, GSD, and FPF (<5 microns) were; 2.9 ± 0.3, 1.9 ± 0.2, and 62.0 ± 1.1 respectively. Topotecan pulmonary deposited doses were 0.13 and 0.79 mg/kg and the IV dose was 0.7 mg/kg. The particle size distribution was measured to be 3.0 µm MMAD. The LCMS analysis showed measurable levels of topotecan throughout almost all time points. The non-compartmental analysis showed a bi-phasic elimination profile from the plasma for IV and inhalation dosing. The inhalation delivery showed increased exposure to the lung tissue for similar doses when compared to IV. The lung tissue exposure approached dose proportionality over the dose range studies. The clearance from the lung was slower following inhalation than IV dose (~ 5 hr. half-life vs 1.2 hr. half-life).

Conclusion: The work presented here demonstrates the feasibility of manufacturing a therapy containing TPT by spray drying. The collected dry powder retained purity, aerosolized in the pulmonary range and was comprised of desirable characteristics by In Vitro assessments. The in vivo PK analysis indicated that when delivered via inhalation and IV topotecan exhibits a bi-phasic elimination profile with increased exposure to the lung tissue following similar dosing IV and inhalation. These results suggest that that with a similar dose the exposure to the lung tissue is increase by a factor of 30. Therefore, inhalation delivery of up to 30-fold lower dose of topotecan than IV could provide similar efficacy for lung cancer and thereby significantly improve toxicity that is greatly limiting the clinical use of this potent anticancer agent.

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3MD.5

Electrospray Functionalization of Titanium Dioxide Nanoparticles with Transferrin for Photodynamic Cancer Therapy.

NATHAN REED, Ramesh Raliya, Rui Tang, Samuel Achilefu, Pratim Biswas, *Washington University in St. Louis*

Electrospray is commonly used to produce macromolecular ions for mass spectrometry, but it has also been studied for generating monodisperse droplets for the synthesis and self-assembly of nanomaterials [1]. Most recently, electrospray has been used to generate nanoparticle standards [2], fabricate solar cells [3], and deliver nanoparticles non-invasively to the brain [4]. The techniques that enable these applications can be extended to many nanomaterials and can efficiently be used to functionalize nanoparticles in a single step. In this work, we functionalize titanium dioxide (TiO_2) nanoparticles with the protein transferrin (Tf) for application in a novel light-based cancer therapy known as Cerenkov radiation induced therapy (CRIT). Tf is a protein that can target the Tf-receptor which is known to overexpress in many types of cancer. Targeted delivery of the nanoparticles can be achieved by coating the TiO_2 with Tf protein. During CRIT treatment, by co-localizing of the PET tracers with nanophotosensitizers in diseased area, the ultraviolet light (UV) generated from β-decay of the radioisotopes can induce the generation of cytotoxic hydroxyl and superoxide radicals from the photosensitizer TiO_2 nanoparticles in vivo to achieve the therapeutic effect [5].

Using electrospray, we have controllably coated Tf on the surface of TiO_2 nanoparticles by drying monodisperse droplets of Tf and TiO_2 before collection. The coating thickness of Tf was tuned by adjusting the precursor concentration of Tf while keeping the TiO_2 number concentration constant. Scanning mobility particle sizer (SMPS) measurements closely match the expected functionalized nanoparticle size for each Tf concentration. Transmission electron microscope (TEM) images further validate this size data and show monodisperse TiO_2 nanoparticles with a coating of Tf after staining. To validate the function of the Tf is unaffected during electrospray processing, the binding affinity of Tf-coated TiO_2 to the Tf receptor was evaluated via MicroScale Thermophoresis (MST).

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3MD.6

Synthesis of Large-Pore Submicron Mesoporous Silica using Salt-Assisted Spray Pyrolysis Method for Controlled Release Drug Delivery. Masoom Shaban, Jalal Poostforooshan, Sarah Reiser, Michael Türk, ALFRED P. WEBER, *TU Clausthal*

Research on mesoporous materials for drug delivery purposes has attracted much attention due to their low cost, non-toxic nature, suitable and adjustable pore diameter, and high specific surface area. However, the irregular bulk morphology of the mesoporous materials obtained by traditional methods is not perfect for drug delivery system. Therefore, to overcome this disadvantage, one strategy is to synthesize submicron mesoporous silica (SMS) with spherical morphology. From a clinical point of view, spherical SMS is widely accepted as the useful drug delivery system, because it can be easily ingested or injected.

In this work, salt-assisted spray pyrolysis was used as a facile aerosol route to obtain large-pore spherical SMS using simple inorganic salts as pore templates and nanocolloidal SiO_2 as building blocks. Significantly, this approach avoids the need for any calcination process and mesoporous particles with high-purity can be produced which is very important in biomedical applications.

The morphology and mesoporous structure of spherical SMS were easily controlled using adjusting salt-to-SiO_2 mole ratio. The textural properties and the topology of the resulting materials were investigated by employing diverse characterization techniques such as scanning mobility particle sizer (SMPS), Micromeretics ASAP 2020, transmission electron microscopy (TEM), and scanning electron microscopy (SEM). Most importantly, porosity was not observed in the particles before exposure to the water, it can be concluded that salt is responsible to induce porosity in the structure. Moreover, wide-angle X-ray diffraction (XRD) and inductively coupled plasma (ICP) results confirmed that there is no residue of salt in the SMS after washing with water.

Then, spray-pyrolysis synthesized spherical SMS was used as a promising carrier for racemic ibuprofen as a poorly water-soluble drug. Ibuprofen is often prescribed to treat e.g. arthritis, fever, and pains, however, its dissolution rate and therewith bioavailability is limited. Therefore, ibuprofen was deposited onto resulting spherical SMS using a controlled particle deposition (CPD) process. This process is a suitable and innovative method for the preparation of dissolution enhancing solid dosage forms without using any additional auxiliary materials.

Finally, it was observed that the ibuprofen loaded-SMS carriers exhibited higher dissolution performances compared to the commercial MCM-41 and SBA-15 type mesoporous silica. Furthermore, the obtained results indicated that there is a direct relationship between specific surface area and obtained drug loading. The SMS carriers with a higher surface area and larger pore volume lead to a higher number of ibuprofen monolayers.

3MS.1

Using Aerosol Photoemission (Ape) for On-Line Process Monitoring of Gas-Phase Particle Modifications.

JANNIS RÖHRBEIN, Alfred Weber, *Clausthal University of Technology*

The surface properties of particulate materials are influencing various powder properties such as flowability, dispersibility, compressibility and general chemical properties like catalytic activity. These characteristics are of significant interest for handling and characterization of those materials. The surfaces of gas-borne particles can be modified in various ways: beside a chemical oxidation, a condensation process might be used to deposit material on their surface. If these condensation processes are to be investigated, it is essential not to change the particle environment during probing.

There are various systems to characterize particle properties such as size, morphology and mass with different degrees between on-line and off-line measurement. However, for the characterization of surface properties of nanoparticles rather involved techniques such as electron spectroscopy (e.g. XPS (X-ray Photoelectron Spectroscopy) or MIES (Metastable Impact Electron Spectroscopy)) have to be employed. These methods suffer from limitations when it comes to (nearly) in situ measurements, i.e. analysis of the particles in the original gas environment, since the electron spectroscopy requires vacuum conditions. When for instance the effect of condensation on the particle surface is to be investigated, vacuum conditions will heavily affect the surface state of the particles due to (partial) evaporation. Additionally, the particle transfer from the synthesis reactor to the vacuum analysing system could lead to sampling artefacts and may be far too complex for process monitoring.

Within this work, a system is presented, which operates at ambient pressure and is based on the photoelectric effect: Singly pre-charged aerosol particles (previously classified by a DMA) are irradiated with light of different wavelengths from an adjustable monochromatic source. The photoelectric effect may remove an electron leading to uncharged particles. Since this method does not require vacuum conditions, the particles can be analysed in the process environment with a simple on-line technique. In addition, in the photoemission measurements morphological effects are taken into account using particles classified according to their mobility with a DMA which is basically given by the particle projection area. Due to the normalization of the photoemission activity to the available surface area the apparatus used here was named Surface-Normalised Aerosol PhotoEmission Sensor (SN-APES).

There already exists extensive, interesting work about Aerosol Photoemission (APE), but the application of APE for process control and monitoring has hardly been addressed. Our approach is the usage of APE for process monitoring of the coating of titanium dioxide with nickel oxide and the diffusion of nickel into the crystal structure of titanium. For this purpose, a commercial photocatalyst (Degussa P25) was dispersed with 1 wt% nickel nitrate in an aqueous solution and spray dried with an atomizer. After drying, the aerosol passed a tube furnace at a temperature representing the process parameter to be investigated. The variation of the product properties with process temperature was analyzed with off-line methods such as TEM, XRD, FTIR and EDX.

By employing aerosol photoemission, it was possible to observe this process on-line, which thereby allows the production of particle material with very defined properties. It was established that the change of the photo-emission behavior of the particles can be related to the surface modification. It turned out that aerosol photoemission, while technically simple, is a very powerful tool for gas phase process monitoring.

3MS.2

Aerosol-assistant Synthesis of Sodium Tungsten Bronze Oxide for UV and IR Shielding. HAO TU, Wei-Ning Wang, Da-Ren Chen, *Virginia Commonwealth University*

The spectrum of solar radiation typically include 10% ultraviolet light (UV), 40% visible light and 50% infrared (IR) light. It is known that UV light is harmful because its high-energy photons can break down the organic bond, potentially resulting in the degradation of matter degradation, eye damage and skin aging. The IR light is the major source of heat radiation. In the summer time, the IR light often raises the temperature in the indoor space when penetrating through windows. The cooling of the indoor space to keep indoor residents comfort consumes much energy. In winters, the indoor heat is partially lost through the IR radiation. Windows with the feature of shielding UV and IR lights while keeping transparent for visible lights have the potential to prevent the residents in the indoor space from the UV radiation while saving energy for cooling the indoor space in summers and heating in winters.

With the properties to absorb the light at in the wavelength less than 370 nm and greater than 800 nm and to be transparent for visible light, sodium tungsten bronze oxide is a perfect functional material for target applications in this study. As a member of tungsten oxides, tungsten bronze oxide is highly resistant to the photochemical corrosion and material degradation and is able to sustain very high temperature, making it suitable for long-term application in hazardous environment. In the literatures, tungsten bronze oxides are synthesized by either hydrothermal, solid reaction or sputtering methods. All of these methods are batched and often require long production time. To the author's knowledge, the above material has not been synthesized by an aerosol route, which is a continuous process to produce materials with high purity and can be easily scaled up in the production.

For the first time, nanoparticles of sodium tungsten bronze oxide were synthesized by an aerosol route in this work. The produced powder of sodium tungsten bronze oxide via the developed aerosol route shows comparable characteristics for the UV and IR light shielding, and the visible light transmittance as the reported one given in literatures. Additionally, a parametric study was also preformed to investigate the effects of the sodium-to-tungsten ratio and operational variables (i.e., the flow rate and heating temperature) on the crystal structure, light absorbance and elemental composition of as-produced powder materials. The details of the developed aerosol route and the result of parametric study will be given in this presentation.

3MS.3

Electric Current-Induced Formation of Defects in Columnar TiO_2 Single Crystals under UV Irradiation for Enhanced CO_2 Photoreduction.

YAO NIE, Pratim Biswas, *Washington University in St. Louis*

Carbon dioxide (CO_2) capture and utilization is a promising potential technology to address global climate change. Photocatalytic conversion of CO_2 into hydrocarbon fuels has attracted abundant research attention in recent years. In this work, columnar titanium dioxide (TiO_2) thin films were synthesized by aerosol chemical vapor deposition (ACVD) method and a new method is reported to generate oxygen vacancies and Ti-related defects (OTDs) in these columnar TiO_2 thin films under UV irradiation with electric current. The defective TiO_2 (TiO_{2-x}) showed a significant enhancement in CO_2 photo-reduction. The substrate, electric current, and electric voltage applied played important roles in affecting the photocatalytic performance. The best performing sample showed the highest CO yield of 375 µmol/g/hr, with an apparent quantum efficiency of 0.045%, which was about 4 times higher than that without current (95 µmol/g/hr), and more than 20 times higher than that of TiO_2 (P25). A recyclability test demonstrated the reversibility of the OTDs in CO_2 photoreduction, with or without an electric current. The formation and healing of OTDs were confirmed by the color change (white to yellow, and back to white) and by HETEM images, UV-vis adsorption, Raman spectra, and XPS spectra. The enhancement of the TiO_{2-x} in CO_2 photoreduction with electric current can be attributed to 1) the narrowed band gap energy, 2) the enhanced chemical adsorption of CO_2, and 3) the better separation of electrons and holes. This study offers new insights into engineering OTDs in TiO_2 for photocatalysis, using an easy and gentle method in ambient environment.

3MS.4

Surface Enhanced Raman Scattering of Silicon Quantum Dots Generated by Laser Ablation. Eisuke Okuchi, TAKAFUMI SETO, Mohamed Abd El-Aal, Makoto Hirasawa, *Kanazawa University*

Silicon quantum dots (Si-QDs, 4 to 12 nm) were fabricated by laser ablation under the helium background gas. Size distribution and the crystallinity of the Si-QDs were controlled by the low pressure differential mobility analyzer (LP-DMA) and the aerosol post annealing process (room temperature to 1273K), respectively. These Si-QDs were deposited on the Cu substrates coated by Ag nanostructure. Raman signal was observed from SiQDs using exciting laser with wavelength of 532nm and power of 0.5 mW with changing the size and annealing temperature (crystal structure) of the Si-QDs. Strongly enhanced Raman signal of Si peak (enhancement factor >10 hold) was observed from the sample prepared by gas phase annealing around the transition temperature of Si crystallization. The enhancement factor decrease with increasing annealing temperature, suggesting a weak interaction between excitation laser (532nm) and nanocrystalline Si (>4nm). The results suggest that the overlapping between the plasmon electric field and the bandgap of Si-QDs might be triggered in the ultrafine silicon nanocrystallines less than 4nm.

3MS.5

Synthesis of Silicon Nanoparticles with Controlled Morphology from Silane Pyrolysis in a Helium Atmosphere and Its Relative Nucleation and Condensation Rates. MIGUEL VAZQUEZ PUFLEAU, Martin Yamane, Pratim Biswas, Elijah Thimsen, *Washington University in St. Louis*

Chemical nucleation is the first step by which gas phase molecules produce solid nanoparticles via chemical reactions. This phenomenon has tremendous technological and environmental relevance, yet, it is still not well understood. Numerous industrial processes including silicon chemical vapor deposition (SiCVD) and silane fluidized bed reactor (SiH4-FBR) are energy intensive processes that could profit significantly from better understanding the initial stages of silicon nanoparticle formation and quantifying the growth rates. However, many difficulties exist to extract experimental kinetic rates in the initial stages of aerosol formation. One of the main challenges is to temporally resolve the kinetics of nucleation and condensation as they occur in the sub millisecond regime. Nevertheless, since the temporal scale of condensation and nucleation are expected to be comparable, the ratio of the speed of both processes can be used to obtain kinetic information.

In this work, a silane pyrolysis flow reactor was used to obtain insights in the nucleation phenomenon. Primary particle size distribution was obtained from transmission electron microscopy (TEM) and supported on X-Ray diffraction (XRD) spectroscopy. These results were contrasted with aerosol online characterizations by scanning mobility particle sizer (SMPS). Interestingly the agglomerate size given by SMPS was not correlated to the reactor temperature but primary particle size distribution was a strong function of it. After finding a suitable temperature where sintering was negligible, primary particle analysis was used to determine the relative condensation and nucleation rates of silane pyrolysis. The results show a relative rate of silicon condensation over nucleation with a dependence to the order of 1.5 with respect to SiH4 precursor. Similarly, the analysis reveals that the total number of formed nuclei is correlated to the initial silane concentration to the power of 2/3. The methodology described here is proposed as a tool to help elucidate the kinetics and morphology of rapidly evolving aerosols made from other materials in a regime where primary particles can be identified and are independent of residence time in the reactor. Such understanding provides experimental information on the nature of the dominant chemical reaction mechanism and can be applied to help engineer silicon nanoparticles for a whole range of applications that require sharp control of primary particle size such as catalysis, battery anodes and biomaterials.

3MS.6

Kinetics of CNT Growth for Aerogelation in FC-CVD Synthesis. FIONA SMAIL, Brian Graves, Adam M Boies, *University of Cambridge*

The potential for macroscopic assemblies of CNTs to create vast improvements in applications where electrical and/or thermal conductivity, low mass, high strength and high toughness are required continues to accelerate research in the field. The most attractive and scalable route to these materials is the one-step continuous synthesis and collection of elastic aerogels of CNTs, using floating-catalyst chemical vapour deposition techniques. The chemistry is driven by an aerosol of iron-based catalyst nanoparticles containing a small amount of sulphur, produced from precursors such as ferrocene (Fe source) and thiophene (S source), which react with hydrocarbon species to grow CNTs.

Recent deconvolution of the process using aerosol sampling techniques has led to new insights relevant to process development, namely:

- The synthesis of long CNTs capable of bundling to form elastic aerogels is driven by the negative slope of the axial parabolic temperature gradient
- The bulk synthesis occurs due to renucleation of Fe-based catalyst particles in the presence of hydrocarbon pyrolysis species
- Renucleation of the Fe-based nanoparticles occurs at higher temperatures and lower Fe supersaturation levels than anticipated as S lowers the Fe nucleation barrier, leading to optimal temperature conditions for CNT growth

To harness the benefits from these recent discoveries for future process scale up, much more information is required about the kinetics of the CNT growth processes in this type of system. While the kinetics of CNT growth in fixed-catalyst bed CVD systems are well characterised, many questions remain about the floating catalyst gas phase synthesis as a) this is a much more difficult system to study b) factors such as diffusion-limitations to growth rates do not apply in the same way. Furthermore, the effect of S, identified since the early days of CNT synthesis as a CNT growth promoted, on the growth rate of CNTs has not been quantified.

This presentation will report the application of aerosol sampling techniques and characterisation of CNT products to the challenge of quantifying CNT growth rates and study how a variety of reaction parameters (catalyst particle size, concentration of S, effect of S-precursor choice, nature of carrier gas, reaction temperature etc) influence the kinetics. The results will aid in optimisation of reactor and process design, to maximise production rates of the macroscopic CNT materials so that their use can be explored and implemented in sectors such as the automotive and aeronautic industries, allowing the benefits of these materials to transform our futures.

3OF.1

Using Oxidation Flow Reactors for Studying the Effect of SOA Aging on Optical Properties and Health Effects. YINON RUDICH, *Weizmann Institute of Science*

Oxidation flow reactors enable studying the effects of aging on various aerosol properties. Here we will present a study on how aging affects the refractive index of non-absorbing SOA under NOx-free conditions. The optical properties of β−pinene and p−xylene SOA produced in an oxidation flow reactor (OFR), were studied using a novel white light-broadband cavity enhanced spectroscopy that measures aerosol extinction as a function of wavelength from 400 to 650 nm. It was found that these SOA are not absorbing in the visible range. The real part of the refractive index (RI), n, for these two types of SOA showed slight spectral dependence. With increased OH exposure, the real part of the refractive index first increased and then decreased, possibly due to an increase in aerosol density and chemical mean polarizability of SOA produced at low OH exposures, and a decrease in mean polarizability of SOA produced at high OH exposures, respectively.

In another study, we investigated the effect of SOA atmospheric aging on cell viability. SOA were formed in an OFR that simulates atmospheric SOA formation and aging dominated by OH radical oxidation under NOx-free conditions. Representative anthropogenic and biogenic volatile organic compounds (naphthalene and α-pinene, respectively) were used. SOA mass and chemical composition were characterized online using a scanning mobility particle sizer (SMPS) and high-resolution time of flight aerosol mass spectrometer (HiRes-Tof-AMS). The SOA were directed to an air liquid interface (ALI) cell exposure system, thus mimicking the deposition of fine particles in the lung. Slightly aged naphthalene-derived SOA (about 2 days) was slightly more toxic than SOA produced from α-pinene. We observed a significant increase in the SOA toxicity following chemical aging for both SOA types, and both aged (10 days) SOA had similar toxicity.

3OF.2

Heterogeneous Oxidation of Brown Carbon Aerosol Diminishes Light Absorption. BENJAMIN SUMLIN, Apoorva Pandey, Michael Walker, Robert Pattison, Brent Williams, Rajan K. Chakrabarty, *Washington University in St. Louis*

Brown carbon (BrC) aerosols are a class of light-absorbing organic aerosols, predominantly emitted from smoldering biomass combustion [1, 2]. BrC aerosols have been shown to absorb near-UV and short visible solar wavelengths which significantly impacts Earth's radiative energy balance. The potential impact of atmospheric processing on the absorptivity of such particles is understudied, and satellite retrieval algorithms and climate models typically treat the optical properties of organic aerosols as constant throughout their atmospheric lifecycle.

Using a Potential Aerosol Mass (PAM) oxidation flow reactor [3], we investigated the effects of photochemical oxidation on the 375-532 nm scattering and absorption characteristics of primary BrC aerosols emitted from smoldering combustion of Alaskan peat, a common fuel for sustained biomass smoldering. Parallel plate activated carbon denuders removed gas phase combustion products, minimizing secondary aerosol formation in the PAM, and a PM_1 cyclone removed particles larger than 1µm. Simultaneous size distribution measurements by a Scanning Mobility Particle Sizer along with a novel Lorenz-Mie theory inversion algorithm [4] facilitated the retrieval of the complex refractive index ($m=n+ik$), and an Aerosol Mass Spectrometer (AMS) was used to obtain the hydrogen-carbon (H:C) and oxygen-carbon (O:C) molar ratios, quantities commonly used to parameterize bulk aerosol composition [5, 6].

Upon oxidation up to approximately 4.5 equivalent atmospheric days, the 375 nm imaginary refractive index and absorption coefficients of BrC particles were found to decrease by ~36% and ~46%, respectively, and the single scattering albedo increased from 0.852±0.005 to 0.898±0.005. From the AMS measurements, we observed an increase in O:C from 0.34±0.01 to 0.40±0.01, suggesting that a transition from functionalization to fragmentation reactions with increasing photooxidation may contribute to the changes in optical behavior. We conclude with simple radiative forcing efficiency calculations that show the effects of atmospheric photooxidation on atmospheric warming attributed to BrC aerosols.

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3OF.3

Ultraviolet and Visible Complex Refractive Indices of Secondary Organic Aerosol Produced by Photooxidation of β-pinene and Naphthalene in the Presence of Nitrogen Oxides.

QUANFU HE, Chunlin Li, Yinon Rudich, *Weizmann Institute of Science*

Atmospheric aerosols strongly influence Earth's energy budget by aerosol-radiation interactions and aerosol-cloud interactions. A large fraction of the submicron aerosols in the troposphere consists of organic aerosol components, of which a large portion is secondary organic aerosols (SOA) originated from biogenic and anthropogenic volatile organic compounds (VOCs). However, the optical properties of SOA are still poorly constrained.

The optical properties of SOA can vary as a function of wavelength, and change with SOA chemical composition. In the real ambient, VOCs are typically mixed with anthropogenic pollutants (e.g. nitrogen oxides, NOx). The addition of NOx during SOA formation introduces alternative oxidation mechanisms, thus modifies the SOA chemical composition and potentially changes the SOA optical properties.

In this study, we produced SOA from β−pinene and naphthalene in the presence of NOx with controlled exposure time in an oxidation flow reactor. The chemical composition of the SOA was characterized by a high-resolution time-of-flight aerosol mass spectrometer. Light extinction data in the ultraviolet-visible range (315-650 nm) measured by a broadband cavity enhanced spectroscopy (BBCES) were obtained. Changes in the complex refractive index due to chemical composition evolution caused by different NOx/VOCs ratios will be investigated. Moreover, the influence of photochemical aging on the SOA optical properties for SOA produced in the presence of NOx will be addressed.

3OF.4

Formation and Aging of Secondary Organic Aerosol from Aromatic Compounds. QI CHEN, Yong Jie Li, Xi Cheng, Yan Zheng, Keren Liao, Ying Liu, Tong Zhu, *Peking University*

Oxidation flow reactors have been widely used to study the formation and evolution of secondary organic aerosol (SOA) over time scales ranging from hours to multiple days of equivalent atmospheric exposure. We deployed a Potential Aerosol Mass (PAM) flow reactor in the laboratory to study the formation and oxidative aging of SOA from typical aromatic precursors such as benzene, toluene and naphthalene. NO_x levels in the PAM chamber were controlled by N_2O injection. Gas-phase precursors and oxidation products are detected by using a proton transfer reaction mass spectrometer and a nitrate-ion chemical ionization time-of-flight mass spectrometer. Non-refractory particle components were detected by using a high-performance time-of-flight aerosol mass spectrometer. Data are compared to ambient observations in Beijing. The mass spectra of highly oxygenated molecules (HOMs) produced by the photooxidation of the three types of aromatic precursors cannot resemble the ambient spectra, suggesting that the majority of HOMs may come from other sources in Beijing. Particle-phase organic nitrate contributes greatly to the SOA mass under conditions of high NO_x. The mass fraction of organic nitrate in organic aerosol is highest for toluene SOA and lowest for naphthalene SOA. However, PAM-generated aromatic SOA shows much less N-containing fragments in the spectra compared to urban SOA in Beijing, implying important brown carbon sources other than aromatic oxidation. The elemental ratios of PAM-generated SOA agree well with the previous findings. As the exposure level increases, the atomic oxygen-to-carbon (O/C) ratios of benzene and toluene SOA increase and the hydrogen-to-carbon (H/C) ratios decrease. In contrast, the H/C ratios of SOA generated from naphthalene photooxidation show an opposite trend with aging, suggesting significant fragmentation.

3OF.5

A High Volume Laminar Flow Reactor to Investigate the Influence of Photochemical Aging on the Health-related Properties of Combustion Emission: Method Characterization and Utilization to Investigate Wood Combustion Emissions. OLLI SIPPULA, Petri Tiitta, Mika Ihalainen, Pasi Yli-Pirilä, Anni Hartikainen, Tuukka Ihantola, Pasi Jalava, Ari Leskinen, Jarkko Tissari, Miika Kortelainen, Heikki Suhonen, Ralf Zimmermann, Maija-Riitta Hirvonen, Jorma Jokiniemi, *University of Eastern Finland, Kuopio, Finland*

One of the main challenges for the assessment of the environmental effects of combustion emissions is their constant transformation in the atmosphere, due to photochemical aging, which may change the health-related toxicological, chemical and physical properties of the emission particles. The devices used to simulate aerosol photo-oxidation include smog chambers and different flow tube reactors. The modern air-liquid cell exposure devices used in toxicological studies, with combined physico-chemical characterizations of aerosol emissions, require relatively high amounts of aerosol sample. To provide sufficient sample flow rates of aged aerosols for these studies, a High-Volume Photochemical Emission Aging Reactor (PEAR), capable of photo-oxidizing high emission concentrations and volumes, was designed and constructed. First, the PEAR was characterized and validated with common precursors for inorganic and organic secondary aerosols. Next, the PEAR-method was compared to a smog chamber using emissions of a logwood-fired stove as a reference. Finally, the device was utilized in connection with air-liquid interface exposure systems, providing information on how aging of combustion emissions influences the biological responses of the exposed lung cells.

The reactor is constructed from stainless steel tube which has 254 nm UV lamps assembled at the inner walls. Ozone and water vapor are added into the reactor to produce OH radicals via photolytical decomposition of O_3. The inlet of the reactor consists of flow diffuser, which is designed to achieve a nearly optimal laminar flow profile in the reactor, when used with the designed flow rates (50-200 lpm). The flow dynamics of the reactor were simulated with the aid of computational fluid dynamics software (ANSYS 15.0, Fluent) to optimize the reactor dimensions and other boundary conditions. According to the gas residence times, measured with CO_2 marker gas, almost fully developed laminar flow profile was achieved at a flow rate of 100 lpm. Consequently wall losses of particles < 50 nm in diameter were very low, below 10%.

In the wood stove experiments diluted exhaust from two different spruce log fired stoves were introduced both into the PEAR and in a 29 m^3 smog chamber (Tiitta et al., 2016). The composition and concentrations of gaseous and particulate species were measured online using HR-PTR-ToF (Ionicon) and SP-AMS (Aerodyne), respectively. Aging in flow tube increased the organic aerosol (OA) mass fraction by 2.1–2.7 times the initial OA mass with OH exposures between 0.8–5.8× 10^{11} molec. cm^{-3}s. OA enhancement ratios were at highest with low OH exposures, which corresponded to 1-2 days of equivalent atmospheric aging at typical boundary-layer OH concentrations. In the smog chamber, the wall-loss corrected OA enhancement ratios were 1.8-2.1, with similar OH exposures, indicating slightly more efficient SOA formation in the PEAR. The AMS mass spectra and calculated oxidation state of OA was similar in PEAR and the smog chamber at similar OH exposures. Furthermore, an intermediate slope of Van Krevelen diagram between -0.6 and -0.7 in ambient oxidation levels indicated similar oxidation reactions (e.g. fragmentation and functionalization) in PEAR and in the smog chamber.

To investigate the role of aging on potential health effects of the emissions, A549 cells were exposed to fresh and aged wood combustion aerosol using an air-liquid interface, in which the particle deposition on the cell surfaces occurs via controlled thermophoretic force. Comparison of fresh and aged aerosol indicated higher inflammation (IL-8), and genotoxic (Comet assay) responses for the aged aerosol, while the cell viability and production of reactive oxygen species (ROS) remained at a similar level. Thus, photochemical aging induced clear changes also in the toxicological properties of the emissions.

This work was funded by the Academy of Finland.

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3OF.6

Secondary Organic Aerosol Yield, Volatility, and Viscosity from Smog Chamber and Flow Reactor Experiments. WYATT CHAMPION, Sarah Suda Petters, Nicholas Rothfuss, Markus Petters, Andrew Grieshop, *North Carolina State University*

Vapor pressure and viscosity of pure organic compounds are controlled by molecular weight and functional group composition. Secondary organic aerosols (SOA) can be mixtures of thousands of compounds. Although it is not obvious that the pure component relationship applies to complex mixtures, one would expect experimental measures of aerosol yield, volatility, and viscosity to relate to experimental measures of chemical composition. These parameters have substantial uncertainties to which laboratory SOA generation systems contribute. Yield experiments utilizing smog chambers introduce bias due to vapor wall losses, and extended aging is difficult due to relatively low oxidant exposures. Yield experiments with flow reactors utilize high oxidant concentrations that may promote fragmentation reactions as opposed to functionalization (leading to higher volatility products and lower yield) (Bruns et al., 2015), and low residence times that may not allow slower processes to occur (e.g., condensation). Here, we apply a combination of methods to probe the ability of each to give insight into the properties of SOA formed from alpha-pinene (α-pinene), and possibly other well-studied precursors, in several laboratory reactors. Objectives of this study are to: 1) compare volatility and viscosity properties of SOA formed in flow reactors to that produced in 'traditional' chamber experiments, and 2) explore relationships between these fundamental aerosol properties.

Organic aerosol mass concentration and chemical composition are measured using an Aerosol Chemical Speciation Monitor. Flow reactor experiments utilize both pure ozonolysis and oxidation driven by low-pressure UV lamps emitting at 254 and 185 nm (OFR-185) oxidation regimes. Smog chamber ozonolysis experiments are also conducted for the same precursors (e.g., α-pinene, naphthalene). For all systems, aerosol yield is quantified using traditional methods. Additionally, volatility distributions are parametrized with the dual thermodenuder (2TD) approach (Saha et al., 2015) in which varied heating perturbations constrain the thermodynamic (heat of vaporization ΔH_{vap}, and saturation concentration, C*) and kinetic (evaporation coefficient, γ_e) properties dictating aerosol volatility. Temperature and RH dependency of viscosity is inferred from the coalescence time scale of synthesized dimers using two differential mobility analyzers of opposite polarity.

Volatility results from 2TD (25-180°C) experiments indicate a substantial presence (>20%) of very low volatility organics (LVOC) in SOA, and evaporation kinetics consistent with moderate kinetic limitation to evaporation (evaporation coefficient ~ 0.1).

Observations of room-temperature dilution-driven evaporation are consistent with the 2TD-derived volatility parameterizations. These distributions are also consistent with others' observations of higher yields and prevalence of LVOCs via chemical analysis. Coalescence experiment results show that the temperature dependence of dry secondary organic aerosol viscosity is similar to that of coal tar pitch, citric acid, and sorbitol. Glass transition temperatures range from –10 to 20°C. Strong correlations of viscosity with O:C and H:C indicate that viscosity is sensitive to changes in composition.

Relationships between oxidation state, yield, volatility distributions, temperature-dependent aerosol viscosity, and enthalpy of vaporization will be explored for single precursor systems at varying levels of oxidation using an oxidation flow reactor at low and high OH exposures. Similarly, the same relationships are explored across systems from different precursors and using different oxidation methods. This work will ultimately allow for more representative estimates of atmospheric organic aerosols in chemical transport models by providing a more robust representation of physicochemical properties of the particles.

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3RA.1

Spatial and Seasonal Variation of Particulate Matter Concentration in Kharagpur-A Mid Sized Town in India. NEHA RANI, B.S Sastry, Kaushik Dey, *Indian Institute Of Technology Kharagpur*

This study represents the spatial and seasonal variation in concentration of particulate matter (PM_{10}, $PM_{2.5}$ and PM_1) of Kharagpur town, India. Kharagpur (220 30' N, 870 72 20' E) is a mid-sized town in Gangetic West Bengal with a population of 207,604. To conduct the study, 32 sites from Kharagpur, were selected and categorized into residential, traffic, commercial and sensitive zone. A one year monitoring has been conducted from October 2014 to September 2015 and a 10 minute data has been taken for each site in every weekend till one year with the help of GRIMM Aerosol spectrometer 1.108. This study gives a detailed account about the annual and seasonal variation of coarse, fine and submicron aerosol concentration throughout the Kharagpur town. The PM data analysis showed that the annual average concentration of PM_{10}, $PM_{2.5}$ and PM_1in study area ranged from 182-365 $\mu g/m^3$, 102-122 $\mu g/m^3$ and 79.81-88.67 $\mu g/m^3$ respectively. The maximum PM10 concentration was found in commercial zone and minimum concentration in sensitive zone. For $PM_{2.5}$ and PM_1, the maximum concentration was observed for traffic zone and minimum was found for residential zone. The seasonal PM data analysis showed highest concentration of PM_{10} (740$\mu g/m^3$) in commercial area and highest concentration of $PM_{2.5}$ (310 $\mu g/m^3$) and PM_1 (237 $\mu g/m^3$) in traffic zone. The PM_{10}, $PM_{2.5}$ and PM_1 concentrations were typically higher during winter season due to prevailing inversion condition causes trapping the pollutants. The significantly high concentration of $PM_{2.5}$ and PM_1 of traffic zone during winter might be the reason of poor dispersion conditions and suspension of fine particles in the ambient air for longer period due to vehicle movement and traffic activities. The submicron fraction of aerosol has been also studied and found that the mean and maximum concentrations of $PM_{2.5}/PM_{10}$ and PM_1/PM_{10} ratios during winter season were slightly higher than summer and monsoon seasons for all the zones. This result also exhibit a condition of poor dispersion and consequently trapping of fine particulates.

3RA.2

Spatial Variation in Aerosol Chemical Composition and Source Contribution in Nepal from Aerosol Mass Spectrometry Measurements. BENJAMIN WERDEN, Michael Giordano, J. Doug Goetz, Khadak Mahata, Narayan Babu Dhital, Nita Khanal, Amit Bhujel, Sagar Adhikari, Siva Praveen Puppala, Maheswar Rupakheti, Prakash Bhave, Robert J. Yokelson, Elizabeth Stone, Arnico Panday, Peter DeCarlo, *Drexel University*

The Kathmandu Valley, an urbanized basin in Nepal, is home to over 3 Million people, and is one of the fastest growing metropolitan areas in South Asia. It is subject to extreme pollution events due to numerous unmitigated localized pollution sources and regional transport from the Indo-Gangetic Plain (IGP). Over 10% of Nepali fatalities are from lung disorders, making it the most common cause of death in the country. Previous field work has studied gas species, wintertime VOCs and PM in the valley. The Nepal Ambient Measurement and Source Testing Experiment [NAMaSTE] of 2015 is the first deployment of a High-Resolution Particle Time of Flight Aerosol Mass Spectrometer (HR-PToF-AMS) in Nepal. Recent measurements in 2017-2018 provide context for spatial analysis of aerosol composition differences and their source contributions in the Kathmandu Valley and Nepal.

The in-situ ambient measurements were made at the Bode site in NAMaSTE 2015. This location is just to the east of Kathmandu. Measurements made in April 2015 were cut short by the 2015 Gorka earthquake so follow-up measurements to complete the dataset were performed in winter of 2017-2018. The winter measurements were made at several other locations in the Kathmandu Valley, and in Lumbini, Nepal in the Indo-Gangetic plain. Differences in aerosol loading and composition are related to the differences in sources and prevailing meteorology at the various sites. Additional gas phase (CO, CO_2, CH_4, H_2O, O_3, NO_x, SO_2,) and particle phase (BC, total PM, filters) measurements were taken in addition to the AMS data and are used to interpret the AMS dataset. Positive Matrix Factorization was used to identify aerosol sources, and chemical signatures were compared to source measurements made during NAMASTE 2015.

The mean concentration of $PM_{2.5}$ in Bode, April 2015 was 83 ± 45 $\mu g/m^3$, which is above the 24 hour WHO exposure threshold of 25 $\mu g/m^3$ and annual continuous exposure limit of 10 $\mu g/m^3$. AMS species show a clear diurnal pattern, with extremely elevated concentrations in the morning. Daily concentration patterns are driven by westerly winds in the late morning to afternoon. This wind is the main method of ventilation, however, it can also introduce pollutants formed over the IGP. Overnight there is confinement by the boundary layer and stagnation due to temperature inversions. This causes an increase in secondary aerosols from an abundance of ammonium, nitrate, and chlorides.

Supplemental AMS measurements at in the southeastern edge of the Kathmandu Valley (Dhulikhel) suggest a strong adabatic/katabatic flow pattern driven by solar gain. The central Kathmandu site, Ratnapark, is heavily influenced by traffic in the city center, with dramatic increases in aerosol loading observed during peak traffic times. Measurements outside of the valley in the IGP (Lumbini) show heavy loading of organics, NH_4, and non-refractory chloride in winter fog episodes.

Localized sources of anthropogenic emissions such as traffic, garbage burning, brick kilns, solid fuel, and dung burning for cooking and agriculture are likely sources of elevated pollutant emissions. Burning of trash and biomass coupled with motor vehicle emissions are a major source of aerosol loading in the measurement region.

3RA.3

Observation of New Particle Formation and Growth for Rural Southwestern New York State. JOSEPH P. MARTO, James Schwab, Fangqun Yu, Gan Luo, *University at Albany, SUNY*

New particle formation (NPF) and growth events are known to introduce significant numbers of particles into the atmosphere which have implications for public health, climate, and atmospheric chemistry. A Fast Mobility Particle Sizer (FMPS) and an Aerodynamic Particle Sizer (APS) continuously measured particle size distributions from 6nm to 20µm to detect changes in particle number and size distribution at Pinnacle State Park (PSP) in rural southwest New York state (42°05′42″N 77°12′54″W) for a year starting March 2017. These measurements indicate dozens of NPF events in a variety of meteorological conditions with most events occurring in the Spring and Fall, and fewer in Winter with a minimal number of events during the Summer. The particle data is combined with collocated measurements of meteorological parameters and numerous gaseous and aerosol properties in an effort to better understand the trigger mechanism and dynamics of nucleation and growth events. Data from the 2017 campaign was compared with observations from briefer field intensives in Summer 2004 and Spring 2009, and a six-month observation period in 2012 to assess any changes in NPF events, specifically in relation to changes in concentrations of chemical precursors. Observational results were also compared to results from a GEOS-Chem model with size-resolved advanced particle microphysics to better interpret the specific chemical and meteorological conditions during these events.

3RA.4

Understanding the High-Resolution Size Distribution of Organic Species over the Indo-Gangetic Plain. NAVANEETH M. THAMBAN, S.N. Tripathi, Bhuvana Joshi, Donna Sueper, Manjula Canagaratna, *IIT Kanpur*

Detailed understanding of the size distribution of organic species in Indo-Gangetic Plain (IGP) at winter period is very important due to their complexity in origin and atmospheric processing. High-Resolution Particle Time of Flight (HR-PToF) size distribution analysis was performed on the High-Resolution Time of Flight Aerosol Mass Spectrometer (HR-ToF-AMS) derived organics data to identify the size distribution of various organic proxies and their relative modes. HR-PToF size distributions of Unit Mass Resolution (UMR) organic proxies (SVOOA, COA and, HOA) show a distinct mode of primary and secondary organic families. The relative abundance of this primary (CH) and secondary (CHO) organic families in a specific UMR proxy can influence its size distribution mode in UMR analysis. The diurnal variation of the mid-modal diameter indicates that the HOA, COA, BBOA are showing a diurnal growth (increase in the mid modal diameter) during the daytime, where, the highly oxygenated LVOOA shows no increase in its mid-modal diameter throughout the day.

3RA.5

Aerosol Characteristics during Intense Crop Residue Burning: A Case Study Over Indo-Gangetic Plain. NANDITA SINGH, Vishnu Murari, Rajesh Kumar Mall, R.S. Singh, Tirthankar Banerjee, *Institute of Environment and Sustainable Development, BHU*

The Indo-Gangetic Plain (IGP), South Asia experiences frequent haze events during post-monsoon (October-November), especially influenced by burning of agricultural residues over upper IGP, and additionally instigate by regional boundary conditions. To understand the effects of biomass burning on regional aerosol characteristics, size-segregated airborne particulates were collected in Varanasi during October to November 2016. Aerosol samples were analyzed for both biomass burning tracers (levoglucosan, K^+, and NH_4^+) and water-soluble ions in coarse mode ($PM_{>2.1}$), finer mode ($PM_{1.1-2.1}$) and accumulation mode (PM<1.1). The concentration of fine particles ($PM_{2.1}$) was found to continuously increase during the period ($PM_{2.1}/PM_{>2.1}$: 0.2-1.5), while fine particles especially dominated during later phase. Biomass burning tracers like levoglucosan were found highest in accumulation mode, followed by fine and coarse mode, and temporal analysis showed the gradual increasing trend similar to particle ratio. The secondary inorganic ions (NH_4^+, NO_3^- and SO_4^{2-}) constituted the major proportion of water-soluble ions and were found highest in $PM_{<1.1}$. A positive correlation was also noted between levoglucosan with K^+ (0.86) and NH_4^+ (0.93) for $PM_{<1.1}$ referring common emission sources. The significant change in fine-mode particle concentration, biomass burning tracers, and secondary inorganic ions in accumulation mode indicate the influence of biomass-burning on fine-mode particulates. MODIS fire count and air-mass back trajectories also indicate possible advection pathways of aerosol from upper to lower Gangetic plain.

Keywords: Levoglucosan, Indo-Gangetic Plain, Biomass-burning, Accumulation mode

3RA.6

One Year Vertically Resolved Optical Closure Study of Aerosol Properties at a Meteorological Tower in Western Europe. Julia Perim Faria, ULRICH BUNDKE, Sebastian H. Schmitt, Thomas F. Mentel, Timothy Onasch, Andrew Freedman, Astrid Kiendler-Scharr, Andreas Petzold, *Forschungszentrum Jülich*

The way airborne aerosols impact climate, either by scattering light or by absorbing it, is well known and documented. The overall effect on the radiation budget depends on three main aerosol characteristics: optical depth, single scattering albedo and backscatter fraction (Haywood and Shine, 1995). Although the aerosol and light interaction mechanism is well understood, the quantification of the fore mentioned impact still presents major uncertainties.

In 2015 a new technology was introduced for measuring single-scattering albedo using a single equipment, the Cavity Attenuated Phase Shift Single Scattering Albedo Monitor (CAPS PMssa), developed by Aerodyne Inc. (Onasch et al., 2015). The instrument, operated in the red spectrum (630nm) has been previously assessed in a multi-instrument optical closure study in the laboratory using controlled particle generation systems and known particle compositions (Faria et al., 2016). The results obtained showed an excellent agreement with proven technology for both absorption and scattering measurement.

Following the laboratory study, the instrument set-up was taken, to a filed campaign, in August 2016, where it sampled ambient air from three different heights, 10, 50, and 120m through sampling lines strategically installed at a meteorological tower located in Jülich, Germany. The instruments used in this campaign are:

- CAPS PMSSA (Aerodyne): Extinction and Scattering Coefficient (630 nm)
- CAPS PMSSA (Aerodyne): Extinction and Scattering Coefficient (450 nm)
- Aurora 4000 (EcoTech): Scattering Coefficient (635, 525 and 450nm)
- PSAP (Radiance Research): Absorption Coefficient (660, 530 and 467nm)
- TAP (Brechtel): Absorption Coefficient (652, 528 and 467nm)
- CPC (GRIMM): Particle Number
- OPC (GRIMM): Particle Size Distribution (655nm)
- AMS (Aerodyne): Chemical Composition.

As the results obtained for the laboratory study, the multi-instrumental optical closure study result during the long term ambient air measuring campaign also showed a good agreement. A few differences were spotted and have been deeper studied, as the Ångstrom exponent from the TAP and PSAP instruments. Regarding the CAPS PMSSA, we have observed that the scattering channel is not stable enough for a long term deployment and needs to be improved.

The chemical information was also analysed by using the data acquired by the AMS system and by the study of the Ångstrom exponent obtained from the multi-wavelength instruments.

The results obtained over the 1 years monitoring campaign have shown many interesting aspects such as the atmospheric aerosol stratification over specific meteorological conditions. It was also possible to observe seasonal trends on aerosol characteristics, such as optical and chemical parameters, size, and load, including vertical distribution.

A few interesting punctual cases were selected to be studied, as the forest fires that occurred in the Iberian Peninsula in October 2017. During week 42, higher extinction, scattering and absorption coefficients were observed. The absorption Ångstrom Exponent average was reduced from 1.52 ± 0.1647, the period before and after week 42, to 1.47 ± 0.1158 during fire period, as expected. This has also been detected and measured by the remote sensing station located in Jülich (JOYCE - Jülich Observatory for Cloud Evolution, Löhnert et al. (2015)).

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4AC.1

Heterogeneous Reaction of Isoprene and Ozone on α-Al2O3 Particles Using Micro-FTIR Spectroscopy. Hongyang Lian, Pang Shufeng, YUNHONG ZHANG, *Beijing Institute of Technology*

Isoprene, a volatile organic compound (VOC), is mainly emitted from biogenic sources with global emissions of about 500 Tg yr-1. Though secondary organic aerosol (SOA) from isoprene ozonolysis through the gas-phase or aqueous reaction has been reported, the research on the heterogeneous reaction of isoprene is lack. As one of the typical oxide minerals, alumina contributes about 15% by mass to the total dust burden in the atmosphere, which has a defined chemical composition and is widely used as model minerals for studying heterogeneous reactions. In order to assess the impact of isoprene ozonolysis on the global SOA budget, it is important to understand heterogeneous reaction of isoprene ozonolysis on the mineral particles and SOA the formation.

The heterogeneous reactions of α-Al2O3 particles with the mixture of ozone (~60 ppm) and isoprene (~50 ppm) were studied as a function of relative humilities (RHs). The reactions were followed in real time using microscopic Fourier transform infrared (micro-FTIR) spectrometer to obtain kinetic data. The results show that ozone leads to rapid conversion from isoprene to carboxylate (COO-) on the surface of α-Al2O3 particles in initial stage. The amount of carboxylate ions on the sample was determined by the infrared absorption calibration curve in order to quantify the carboxylate ions formation rate d[COO-]/dt in terms of the reactive uptake coefficient. The reaction is sensitive to RHs and surrounding water significantly suppresses the formation of the carboxylate ions. For the isoprene ozonolysis reaction on the α-Al2O3 particles, the reactive uptake coefficient is strongly enhanced by over a factor of four as the RH decreases from 87% to 28%. The results imply that the Criegee intermediates generated from isoprene ozonolysis have low reactivity toward water resulting in the suppression of SOA formation.

4AC.2

Methylthreonic, Methylerythronic, and Methyltartaric acids: Highly Oxygenated Markers for Isoprene Secondary Organic Aerosol Aging. MOHAMMED JAOUI, Rafal Szmigielski, Nestorowicz Klara, A. Kolodziejczyk, K.J. Rudziński, W. Danikiewicz, Michael Lewandowski, Tad Kleindienst, *EPA/ORD/NERL*

We investigate the formation of new highly oxygenated molecules (HOMs) associated with secondary organic aerosol (SOA) originated from isoprene photooxidation and ozonolysis under a wide range of conditions. SOA was generated by the oxidation of isoprene/air mixtures in the presence of NOx, H2O2, methyl nitrite, or ozone. The effect of relative humidity, acidity, and OH radical scavengers (ozonolysis experiments) on the formation of these HOMs was investigated. Using a detailed analysis of mass spectra obtained from GC-MS of silylated derivatives in EI and CI modes, and UPLC/ESI/QTOF HRMS, and collision-induced dissociation in positive and negative modes, we identified not only typical isoprene products, but also six HOMs: 2-methylerythronic acid (2MeTrA), 3-methylerythronic acid (3MeTrA), 2-methylthreonic acid (2MTrA), 3-methylthreonic acid (3MTrA), L-methyltartaric acid (L-MTA), and D-methyltartaric acid (D-MTA). We confirmed their structure by synthesizing them in our laboratory. Isoprene HOMs with O/C ratio of 1 and 1.2 were not detected in the presence of OH scavenger during ozonolysis, suggesting OH radicals are important in isoprene HOMs formation. The presence of these HOMs in the gas and particle phase simultaneously provides evidence of their gas/particle partitioning. The occurrence of these HOMs in ambient aerosol collected during the past 15 years in several locations in USA and Europe provide direct molecular evidence of isoprene aging processes in ambient aerosol. For example, the average concentrations of 2MeTrA + 2MTrA, 3MeTrA + 3MTrA, and L-MTA + D-MTA in Duke Forest samples were 0.42, 0.11, and 3.49 ng m-3. We also present results from time-resolved experiment of gas and particle products, where 4-hydroxy-3-methyl-but-2-enal, and 4-hydroxy-2-methyl-but-2-enal are proposed as possible precursors to HOM formation.

Keywords: Isoprene, HOMs, methyltreonic acid, methylerythronic acid, methyltartaric acid, secondary organic aerosol.

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4AC.3

The Effect of Temperature on Secondary Organic Aerosol Formation from Evaporated Fuels and Aromatic Compounds under Daytime and Nighttime Conditions. JEFF BEAN, Shaokai Gao, Terry Lathem, *Phillips 66*

Secondary organic aerosol (SOA) is an important contributor to ambient concentrations of particulate matter. SOA is formed from oxidation of anthropogenic and biogenic volatile organic compounds (VOCs) in the atmosphere. Chemical transport models (CTMs), such as the Community Multi-scale Air Quality Model (CMAQ) and the Comprehensive Air Quality Model with Extensions (CAMx), provide estimates of SOA formation based on data acquired from environmental chamber experiments and ambient measurements. The model parameters used to calculate SOA must be continuously evaluated and updated to incorporate advances in SOA research. It is important to evaluate model performance for multiple VOC precursors and across a variety of environmental conditions.

The present study compares SOA formation in 7.5 m^3 environmental chambers with box model predictions for evaporative emissions of commercial fuels (gasoline and diesel) and single component aromatics. Experiments were conducted across a range of temperatures as well as under both daytime and nighttime oxidative conditions. Experiments were modeled using the SAPRC box model with the SAPRC07 chemical mechanism and the AERO6 SOA parameters, similar to the SAPRC07TC_AE6_AQ mechanism used by CMAQ version 5.1. Key results from comparisons of modeled and experimental SOA formation at varying temperatures and oxidative conditions will be presented. These results highlight areas where further improvements are needed to increase model accuracy.

4AC.4

Characterization of Isoprene-derived Secondary Organic Aerosols at a Rural Site in North China Plain with Implications for Anthropogenic Pollution Effects.

JIANJUN LI, Gehui Wang, *Institute of Earth Environment, CAS*

Isoprene is the most abundant non-methane volatile organic compound (VOC) and the largest contributor to secondary organic aerosol (SOA) burden on a global scale. In order to examine the influence of high concentrations of anthropogenic pollutants on isoprene-derived SOA (SOAi) formation, summertime PM2.5 filter samples were collected with a three-hour sampling interval at a rural site in the North China Plain (NCP), and determined for SOAi tracers and other chemical species. RO2+NO pathway derived 2-methylglyceric acid presented a relatively higher contribution to the SOAi due to the high-NOx (~20ppb) conditions in the NCP that suppressed the reactive uptake of RO2+HO2 reaction derived isoprene epoxydiols. Compared to particle acidity and water content, sulfate plays a dominant role in the heterogeneous formation process of SOAi. Diurnal variation and correlation of 2-methyltetrols with ozone suggested an important effect of isoprene ozonolysis on SOAi formation. SOAi increased linearly with levoglucosan during June 10-18, which can be attributed to an increasing emission of isoprene caused by the field burning of wheat straw and a favorable aqueous SOA formation during the aging process of the biomass burning plume. Our results suggested that isoprene oxidation is highly influenced by intensive anthropogenic activities in the NCP.

4AC.5

IEPOX Uptake Changes Particle Morphology and Viscosity. NICOLE OLSON, Ziying Lei, Rebecca Craig, Yue Zhang, Yuzhi Chen, Jason Surratt, Andrew Ault, *University of Michigan*

In atmospheric particles, organics become mixed with inorganic species via gas-phase oxidation of volatile organic compounds (VOCs) with subsequent condensation of the low-volatility products, such as isoprene epoxydiols (IEPOX), key products of isoprene photo-oxidation, which leads to the formation of secondary organic aerosol (SOA). Chamber and field studies have observed complex physicochemical properties of SOA, such as liquid-liquid phase separations (LLPS) and viscous or glassy organic phases, that inhibit reactive uptake of gaseous species, lower partitioning of chemical species from particle to gas phase, and lower the relative humidity (RH) at which particles undergo efflorescence and deliquescence. To determine the impact these complex morphologies have on the formation of IEPOX-derived SOA, laboratory experiments were conducted by exposing gaseous IEPOX to acidic ammonium sulfate particles coated with α-pinene and toluene SOA at a range of RH (15-50%).To determine individual particle morphology and viscosity, single-particle microscopic and spectroscopic techniques, including scanning electron microscopy coupled with energy dispersive x-ray spectroscopy (SEM-EDX), Raman microspectroscopy, and atomic force microscopy (AFM), were used. After IEPOX uptake, changes to particle morphology and an increase in particle viscosity were observed, which decreased additional IEPOX uptake and limited subsequent particle growth. Particle phase and viscosity determination is necessary to more accurately predict atmospheric fate of ambient aerosols, and the effect aerosols have on heterogeneous (multi-phase) chemistry, climate, and air quality.

4AC.7

A Simplified Parameterization of Isoprene Epoxydiols Derived Secondary Organic Aerosol (IEPOX-SOA) for Global and Climate Models. DUSEONG JO, Alma Hodzic, Louisa Emmons, Eloise Marais, Zhe Peng, Weiwei Hu, Pedro Campuzano-Jost, Jose-Luis Jimenez, *University of Colorado Boulder*

Isoprene is the most abundant non-methane volatile organic compound in the atmosphere and substantially contributes to secondary organic aerosol (SOA) concentrations globally. Isoprene epoxydiols derived SOA (IEPOX-SOA) is thought to contribute the dominant fraction of total isoprene SOA. IEPOX-SOA depends on aerosol pH and other properties, and cannot be calculated accurately with lumping SOA schemes such as two-product and volatility basis set approaches. Recent modeling studies have found generally good agreement between simulated and observed IEPOX-SOA after including detailed isoprene chemistry. However, these models require high computational cost including the calculations of chemistry, deposition, and transport processes of intermediates (e.g. isoprene peroxy radicals, ISOPOOH, IEPOX, etc.). This makes it difficult to include into climate models for long-term studies. For similar reasons, the latest version of the GEOS-Chem model includes a fixed 3% yield of SOA from isoprene for most model applications, in order to avoid the extra computational cost of the full mechanism. Here we present a simplified parameterization for IEPOX-SOA simulation, based on an approximate analytical solution of the relevant portion of the isoprene chemical mechanism. The IEPOX-SOA yield and formation timescale can be directly calculated using the current model fields of oxidant concentrations, NO, aerosol pH and other key properties, and dry deposition rates. Therefore, the parameterization does not require the simulation of the intermediates with maintaining chemical fidelity for simulating IEPOX-SOA. The simulated IEPOX-SOA with the parameterization shows R^2 of 0.96 in comparison to that with the full chemistry in terms of temporal (timeseries in source region) and spatial (global map) variations. Detailed methodology and evaluation results of the parameterization will be discussed.

4AC.8

Compositional Analysis of Aerosols and Rain Water during Weak South-west Monsoon Period. PRADHI RAJEEV, Prashant Rajput, Gyanesh Kumar Singh, Vikram Choudhary, Amit Kumar Singh, Tarun Gupta, *Indian Institute of Technology Kanpur*

Particulate matter (PM) loading during South-west (SW) monsoon is significantly less over the Indo-Gangetic Plain (IGP) due to frequent wash out by wet precipitation and high convective mixing [Temp: ~ 40 °C; wind speed: ~8 m/s]. However in year 2015, weak SW-monsoon due to El-Niño and positive phase of Pacific Decadal Oscillation (PDO) has resulted in less rainfall (~ 375 mm) than usual (~ 900 mm) over the IGP region. Thus, low wet precipitation has facilitated to assess several characteristic features of aerosols and rain waters during the SW-monsoon. We have conducted a study in the central IGP during SW-monsoon to assess chemical characteristics of ambient atmospheric aerosols ($PM_{2.5}$; n= 42; 42.2 ± 22.4 μg/m3) and individual rain water samples (pH: 6.4−7.6; n = 15). Different chemical constituents like organic carbon (OC), elemental carbon (EC), water-soluble organic carbon (WSOC), water-soluble inorganic species (WSIS), water-soluble total nitrogen (WSTN) and metals have been studied in aerosols. However, in rain water samples, pH, electrical conductivity, WSOC, WSIS and WSTN have been assessed. In aerosol samples, the contribution of secondary inorganic species viz. SO_4^{2-}, NH_4^+ and NO_3^- in WSIS were found to be predominant. In a sharp contrast, HCO_3^- and Ca^{2+} constituted the major fraction of total WSIS in rain waters. Characteristic mass ratios among ionic species in rain waters and aerosol samples suggest that below-cloud scavenging is predominant mechanism of aerosols wash out over the region. The mass contribution of total carbonaceous aerosols (TCA), mineral dust (MD) and WSIS in PM2.5 was found to be 22%, 37% and 35%, respectively. Higher contribution of mineral dust in $PM_{2.5}$ is attributable to significant upliftment of mineral aerosols due to drier weather condition and high wind speed. Mineral dust characteristics in $PM_{2.5}$ have been assessed systematically utilizing elemental ratios of major crustal metals i.e. Fe/Al, Ca/Al and Mg/Al. Our study documents that rain waters over the IGP is alkaline in nature and provides a field-based evidence that fine fraction mineral dust favors the uptake of secondary species like nitrate.

4AC.9

A Multi-Season Investigation of Non-Combustion-Related Emissions of Gas-Phase Organic Compounds in Two Major U.S. Cities. PEEYUSH KHARE, Jenna Ditto, Taekyu Joo, Nga Lee Ng, Drew Gentner, *Yale University*

Emissions from combustion-related sources have historically dominated urban air pollution but non-combustion emissions are now playing an important role in determining the U.S. urban air quality (Khare and Gentner (2017), ACPD). Despite their growing significance, the magnitude, composition, secondary organic aerosol- and ozone- formation potential of non-combustion emissions in the atmosphere are largely understudied. In this study, we present results from our summer and winter air quality measurements in New York City, NY and Atlanta, GA with particular attention to the influence of non-combustion emissions. Gas- and particle-phase samples were collected at the New York State Department of Environmental Conservation (NYSDEC) site located in Queens, NY, a Manhattan facing residential building in Harlem, NYC and, at the Southeastern Aerosol Characterization (SEARCH) site near downtown Atlanta, GA. The collected samples were analyzed using traditional GC-MS, as well as using a very high resolution tandem mass spectrometer (i.e. MS×MS) employing atmospheric pressure chemical ionization and electrospray ionization inline with gas and liquid chromatographic separations, respectively. This provided molecular-level and structural characterization over a broad polarity and volatility range. A diverse suite of emitted organic compounds spanning across a wide polarity and volatility range is studied with special focus on under-characterized halogen- or phosphorus-containing organic pollutants and other intermediate volatility and semi-volatile organic compounds (IVOCs and SVOCs) whose direct and indirect health impacts are well documented. All prominent isomers are identified and reported, and are characterized by their accurate molecular formula, structural elements, and volatility. We report information on the range of urban concentrations of all measured compounds for comparison between the cities and seasons. Concentrations of each compound of interest are tested for least-squares correlation with CO concentrations, a common method for calculating emission since urban emissions of CO are mostly anthropogenic primary emissions, and provide a robust way to compare emissions between cities and scale up emissions with validated CO emissions inventories. Total urban emissions and individual concentrations are summarized by carbon number, compound class, and functionalities across the entire volatility span up to SVOCs. Measured compounds at each site are statistically evaluated for likely co-emissions or covariance via automated full dataset regressions in Igor Pro. We also collected and chemically characterized gasoline and diesel fuel samples from each city and season to constrain the contribution of motor vehicles to observed emissions using source apportionment methods. Our study aims to resolve major knowledge gaps in emissions inventories that are necessary for air quality models and comprehensive air quality policies in an era where non-combustion sources are emerging as key, prevalent factors in urban air quality.

4AC.10

Automated Organic Aerosol Measurement with Quartz Filter-based Thermal Desorption Gas Chromatography Mass Spectrometry (TAG). HAIXIA REN, Mo Xue, Zhaojin An, Wei Zhou, Jingkun Jiang, *Tsinghua University, Beijing, 100084, China*

Rapid characterization and high chemical resolution of organic compounds in atmospheric particulate matter are required in aerosol research, especially when revealing the sources of primary organic aerosol, the formation of secondary organic aerosol and atmospheric evolution of organic aerosol. Real-time characterization is preferable considering the variation and lability of organic aerosol, although it can be very challenging due to the chemical complexity of aerosol, especially characterization at molecular level. In-situ thermal desorption aerosol gas chromatography (TAG) was previously developed to characterize organics in aerosols at molecular level. Briefly, aerosols are collected in a collection cell, then organics in aerosols are thermally vaporized and captured in a cooled trap, finally injected into gas chromatograph (GC) for analysis. However, previously reported either stainless steel impactor or metal-fiber filter based TAG has high risk of residue accumulation, especially under severe particulate matter loading that is frequently encountered in polluted atmospheric environment.

In this study, a quartz filter based TAG, which can be readily disassembled and allows filter replacement, has been developed and evaluated using C7-C40 n-alkanes. The developed device is composed of a quartz filter collection cell, temperature and pressure control system, and combined with commercial gas chromatography mass spectrometry (GCMS) for evaluation. The thermally desorbed organics were trapped by the analytical column. C11-C40 with boiling point from 196 – 525°C was detected with residues of less than 1% and demonstrated repeatability of less than 10% except for C11, C12, and C40. Considering the complexity of organic aerosol, the device was hyphenated with two dimensional gas chromatography (GC´GC-MS) for analysis, and the analytical performance was validated by alkanes, polycyclic aromatic hydrocarbons, sterols, acids, etc. The developed instrument was deployed for hourly in-situ organic compounds analysis of ambient PM2.5 in Beijing, and organic aerosol emissions from residential solid fuel combustion. Results from these field studies will be discussed.

4AC.11

Size and Composition Dependent Seed Particle Growth by α-Pinene Ozonolysis. JUSTIN KRASNOMOWITZ, Michael J. Apsokardu, Chris Stangl, Shanhu Lee, Murray Johnston, *University of Delaware*

Biogenic secondary organic aerosol (BSOA) is a key contributor to particle formation and growth in the atmosphere. In principle, growth mechanisms and rates can be both seed particle size and composition dependent. This work utilizes a flow tube reactor with a 4 minute residence time to study these dependencies. Experiments performed to date were done by exposing monodispersed ammonium sulfate seed particles to varying amounts of highly oxidized molecules (HOMs) produced by α-pinene ozonolysis at low relative humidity (10%) and room temperature. Experiments were performed by first introducing monodispersed ammonium sulfate seeds (40, 60 or 80 nm in diameter) into the flow tube along with a low ozone mixing ratio. Next, α-pinene (14 ppbv) was added to begin HOM production. The ozone mixing ratio was then systematically increased from 30 to 300 ppbv during the course of the experiment to increase the average HOM mixing ratio, which caused an increasing amount of seed particle growth. Particles exiting the flow tube for each increment of ozone mixing ratio were characterized with SMPS (size distribution), NAMS (elemental composition) and ESI-HRMS (molecular composition). To a first approximation, particle growth rates were found to be independent of seed particle size and increased linearly with increasing ozone mixing ratio. The measured growth rates were consistent with a kinetic growth model based on the average HOM mixing ratio in the flow tube for each ozone increment. If anything, the kinetic model slightly underestimated the measured growth rate, suggesting that some multiphase chemistry may have occurred in addition to HOM condensation. Current and planned work will explore the effects of seed particle phase (dry vs. wet ammonium sulfate, organic vs. inorganic seed composition) as well as extend these measurements to smaller seed particle sizes.

4AC.12

Application of Spin Traps to Detect Reactive Intermediates and Reactive Oxygen Species in Secondary Organic Aerosol. STEVEN J. CAMPBELL, Chiara Giorio, Peter J. Gallimore, Svetlana Stevanovic, Branka Miljevic, Steven Bottle, Zoran Ristovski, Markus Kalberer, *University of Cambridge*

The chemical composition and evolution of secondary organic aerosol (SOA) in the atmosphere represents one of the largest uncertainties in our current understanding of air quality. Despite vast research, the toxicological mechanisms relating to adverse human health effects upon exposure to particulate matter are still poorly understood. Studies suggest that particle bound reactive oxygen species (ROS) are a major contributor to observed health effects associated with exposure to ambient particulate matter. ROS is an umbrella term, which encompasses a large range of species including peroxides, oxidised organics, organic radicals and the transition metal-induced formation of peroxides and radicals. Several chemical assays are available for ROS detection, all of which are sensitive to a certain fraction of ROS species in aerosol. However, the role of radicals and reactive intermediates in both the formation and ageing of aerosol, as well as their contribution to the health-relevant properties of ambient aerosol, at present remains highly uncertain. We recently developed a technique to quantify organic radicals in the gas phase by stabilising them with spin traps, and subsequent analysis using various mass spectrometry techniques.[1] Recently, a study by Stevanovic *et al.*[2] introduced the profluorescent spin trap BPEAnit (9,10-*bis*-(phenylethynyl)-anthracene-nitroxide) which has been shown to be capable of quantifying particle-bound radicals in aerosol generated from the combustion of biomaterial and fuel.

In this work, BPEAnit is applied to study the concentrations of particle-bound radicals in SOA. Radical concentrations were estimated for SOA generated from the ozonolysis of α-pinene, β-caryophyllene and limonene in a flow tube, to probe the assays response to SOA formed from biogenic precursors typically found in the atmosphere. SOA is captured in an impinger containing the BPEAnit/DMSO assay, before subsequent analysis using fluorescence spectroscopy. Additionally, the BPEAnit spin trap assay allowed the design of experiments to probe the lifetime of radical species in α-pinene SOA, producing first estimates of organic radical decay in SOA. A pseudo-1st order rate constant of $k = 7.3 \pm 1.7 \times 10^{-3}\ s^{-1}$ was derived, implying a radical lifetime on the order of minutes in fresh α-pinene SOA.

Furthermore, building on our recent work by Giorio *et.al.*,[1] the spin trap PBN (*N*-*tert*-butyl-α-phenylnitrone) was used to trap Criegee intermediates (CIs) present in the aerosol phase, with the resulting adducts analysed using high performance liquid chromatography high-resolution mass spectrometry. Experiments were conducted with this method using SOA generated from β-caryophyllene ozonolysis in a flow tube, demonstrating the technique's unique capability to detect multiple CIs present in SOA. Criegee intermediate concentrations in the aerosol phase were measured to be 4.5 ± 0.7 ng [CI]/µg SOA, providing the first estimate of condensed phase CI concentrations in SOA.

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4AC.13

The Effect of Gasoline Car Exhaust on the Photochemistry of α-Pinene. EETU KARI, Liqing Hao, Sini Isokääntä, Arttu Ylisirniö, Ari Leskinen, Pasi Yli-Pirilä, Celia Faiola, Santtu Mikkonen, Annele Virtanen, *University of Eastern Finland*

Biogenic and anthropogenic emission sources emit particles and volatile organic compounds (VOCs) into the atmosphere. Due to the presence of biogenic and anthropogenic emissions in many locations at the same time, potential interactions between the compounds emitted from these two sources has raised particular scientific interest. To clarify the biogenic-anthropogenic interactions, controlled laboratory studies with real emission sources are required. The laboratory studies with real emission sources represent better the complexity of these interactions than the studies with only pure standards, but still allow controlled conditions to investigate the processes in systematic way. In this work, we conducted an environmental chamber study to explore possible anthropogenic-biogenic interactions between a modern gasoline car (VW Golf 1.2 TSI) exhaust and α-pinene under atmospherically relevant conditions.

To investigate the effect of gasoline car exhaust on α-pinene photochemistry, we conducted three kinds of experiments: 1) experiments with only diluted gasoline car exhaust, 2) experiments with α-pinene and diluted gasoline car exhaust, 3) experiments with α-pinene and ammonium sulphate (AS) particles. In experiment type 3) the VOC/NOx ratio was adjusted so that it was comparable to experiment types 1) and 2). Both gas- and particle phases were monitored using Proton-Transfer-Reaction Time-of-Flight Mass Spectrometer (PTR-ToF-MS), Chemical Ionization Atmospheric Pressure interface Time-of-Flight Mass Spectrometer (CI-APi-ToF-MS) with acetate ionization, Aerosol Mass Spectrometer (SP-AMS), and Scanning Mobility Particles Sizer (SMPS).

We found that depending on the experiment in experiment type 1) gasoline car exhaust produced SOA and the formed SOA mass varied due to the changes in exhaust gas composition. From PTR-ToF-MS data, we were able to identify 18 SOA precursors whose reactions with OH-radicals explained 17%-64% from the observed SOA formation depending on the experiment indicating that some important SOA precursors, such as SVOCs, were not detectable by PTR-ToF-MS. In the experiment type 2) we were able to separate 4 factors from particle phase data measured by AMS using positive matrix factorization (PMF) method: HOA factor that was originated from car exhaust, mixed LVOOA factor that was produced by SOA originated from the photochemistry of car exhaust and α-pinene, α-pinene SVOOA factor, and α-pinene LVOOA factor. From PMF results we were able to estimate the formed SOA mass from car exhaust in experiment type 2), when both car exhaust and α-pinene were present in the chamber during the photo-oxidation. After subtracting car exhaust SOA from α-pinene SOA, we were able to conclude that the other compounds than NOx in gasoline car exhaust did not have a significant effect on SOA yield of α-pinene, and that SOA formed from α-pinene photo-oxidation dominated the total SOA mass in each experiment.

The results of this study indicate that in environments, where gasoline car exhaust is mixed with α-pinene, the photochemistry of α-pinene is significantly affected only by NOx. These results demonstrated also the need to study the car exhaust emissions with the instruments that can quantitatively measure SVOCs in order to fully understand the SOA formation from gasoline exhaust.

4AC.14

Formation of Secondary Organic Aerosol from Photo-Oxidation of Benzene. SEBASTIAN H. SCHMITT, Thomas F. Mentel, Jürgen Wildt, Einhard Kleist, Iida Pullinen, Ying Liu, Baolin Wang, Defeng Zhao, Astrid Kiendler-Scharr,
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Understanding the formation of secondary organic aerosol (SOA) is crucial for estimating its impact on the earth's climate as well as on human health and the development of future mitigation and adaptation strategies. The potential of SOA formation from the oxidation of a certain volatile organic compound (VOC) is often expressed as the SOA mass yield being the ratio of formed SOA mass and consumed VOC. Typically, this is determined from single VOC oxidation experiments in atmosphere simulation chambers. Even though the SOA mass yield is an easy to calculate quantity, caution has to be taken to accurately determine it in a specific atmosphere simulation chamber.

Within this study the formation of SOA from the photo-oxidation of benzene was systematically studied in the Jülich Plant Atmosphere Chamber (JPAC) at the campus of Forschungszentrum Jülich GmbH. JPAC is a continuously stirred tank reactor made of borosilicate glass and it was operated with a typical mixing time of 2 minutes and a residence time of 45 minutes. The oxidizing conditions (OH concentrations, NO_x concentrations) were systematically altered in order to study their respective influence on SOA mass formation. A combination of Scanning Mobility Particle Sizer (SMPS), Aerosol Mass Spectrometry (AMS) and Chemical Ionization Mass Spectrometry (NO_3-CIMS) provided novel insights into the formation process of secondary organic aerosol.

The loss of oxidized SOA precursor molecules to the walls of the reaction chamber must be considered for retrieving the most accurate SOA mass yield. For this purpose an already existing correction function was extended, in order to take into account semi-volatile organic compounds with lifetimes longer than the residence time of the chamber. In order to accurately determine this correction function, ammonium sulfate seed aerosol was used to alter the fraction of SOA precursors lost to the chamber wall systematically. Here, the organic fraction of SOA was determined with the AMS while the NO_3-CIMS provided measurements of the oxidized SOA precursors in the gas phase.

After correction of unseeded experiments for wall loss of SOA precursor by the modified correction function, the SOA mass yield of benzene was found to be 28±13 %. A similar yield (29±4 %) was obtained by using seed aerosol with the uncertainty being largely reduced in presence of seed aerosols. Within the accessible range of the steady state measurements, no dependence of the benzene SOA mass yield on OH could be detected. Also, NO_x had no significant influence on the SOA mass yield from benzene photo-oxidation. However the formation of new particles (nucleation) was strongly suppressed by increasing NO_x concentrations.

A comparison of the obtained SOA mass yield results with literature data shows a large variation, likely due to the sensitivity to the operational conditions of the different experiments.

4AC.16

Characterization of Particulate Matter Sources in Summer Using High-Resolution Aerosol Mass Spectrometry in San Antonio. FANGZHOU GUO, Benjamin Schulze, Alexander Bui, Henry Wallace, James Flynn, Matthew H. Erickson, Sergio Alvarez, Alex Kotsakis, Subin Yoon, Sascha Usenko, Rebecca Sheesley, Robert Griffin, *Rice University*

Currently the seventh most populous city in the United States and the second most populous city in Texas, San Antonio has been one of the most rapidly growing large cities in the country over the past decade. As evidenced by an ozone design value in violation of the federal threshold for a recent three-year period (2014-2016), the city suffers from poor air quality. To understand the sources of particulate matter (PM) that contribute to the degradation of San Antonio's air quality, we assembled and deployed a mobile air quality laboratory and operated it in two locations in the southeast (Traveler's World RV Park) and northwest (University of Texas at San Antonio campus) of downtown San Antonio from May 2 through May 30, 2017. Chemical characterization of non-refractory submicron PM (NR-PM1) at high time resolution was conducted using an Aerodyne high-resolution time-of-flight aerosol mass spectrometer (HR-ToF-AMS). Additional measurements included meteorological parameters, trace gas mixing ratios (of ozone, total nitrogen oxides, total reactive nitrogen, carbon monoxide, and volatile organic compounds), and off-line speciation of PM collected using filters. This is the first time that detailed real-time aerosol measurement results have been reported from San Antonio.

From the preliminary results, organic and sulfate aerosols dominated the total aerosol burden, averaging 5.42 mg/m3 (54% of the total mass) and 3.43 mg/m3 (31% of the total mass), respectively. The average concentrations of ammonium (1.21 mg/m3; 11%), nitrate (0.33 mg/m3; 3.6%), and chloride (0.04 mg/m3; 0.4%) were relatively smaller throughout the campaign period. Total aerosol mass concentrations displayed two high-loading periods (May 9-12 and May 27-29), with the first one propelled by both organics and sulfate and the second one dominated by sulfate aerosols.

Positive matrix factorization, in conjunction with meteorological and trace gas data, will be used to apportion the organic portion of NR-PM1 to various types of organic aerosol, including proxies for primary and secondary organic aerosol. Preliminary results indicate atypically large sulfate aerosol plumes; the relative contribution of biogenic and anthropogenic sources to this sulfate will be quantified. In addition, large spikes of biomass burning organic aerosol appear to originate from agricultural fires in Central America. This combination of data will allow us to estimate the fraction of PM in San Antonio in summer that is local and anthropogenic, potentially providing guidance for development of emission control strategies.

4AC.17

Hygroscopic Behaviours of Inorganic/Organic Mixtures Including Ammonium sulfate, Dicarboxylic Acid and Oligomer.

HICHEM BOUZIDI, Andreas Zuend, Jakub Ondrácek, Jaroslav Schwarz, Vladimír Ždímal, *Institute of Chemical Process Fundamentals of the CAS*

Aerosol particles are an important atmospheric constituent, influencing global climate. The hygroscopic growth behaviour of aerosol particles is one of the important parameters controlling these climate effects. Atmospheric aerosol particles are generally complex mixtures of a diversity of inorganic constituents and organic compounds. In many regions, organic aerosol dominates the ambient aerosol mass. It is well established that high-molecular-weight organic compounds like oligomer with molecular masses ranging from 200 to 1600 $gmol^{-1}$ [1], represent an important fraction in atmospheric aerosols, but their interactions with other inorganic/organic, and atmospheric water vapour are not well understood. Moreover, single particle measurements suggest that organic and inorganic constituents are internally mixed in particulate matter [2]. Therefore, Non-ideal interactions between the organic and inorganic aerosol fractions affect water uptake and solubility, may induce Liquid-liquid phase separation (LLPS) into an organic-rich and an aqueous electrolyte phase (phase separation), may affect efflorescence and deliquescence behaviour, and alter the gas/particle partitioning of semi-volatile compounds [3-4]. The presence or absence of LLPS in aqueous mixtures can be computed using a liquid-liquid equilibrium model [3].

Here, the hygroscopic properties of submicron particles under subsaturated relative humidity (RH), composed of ammonium sulfate, dicarboxylic acids including oxalic acid (OA), malonic acid (MA), and oligomer Poly(Ethylene-Glycol) (PEG-300 $(\text{-CH2OCH2-})_n$) with various mixtures and mass ratios are investigated in a laboratory study using a Hygroscopicity Tandem Differential Mobility Analyzer (HTDMA). Those constituents correspond to materials found in the atmosphere in great abundance and, therefore, particles prepared in this study should mimic atmospheric mixed-phase aerosol particles.

The experimental data are compared with predictions from Zdanovskii-Stokes-Robinson (ZSR) mixing rule and Aerosol Inorganic-Organic Mixtures Functional groups Activity Coefficients (AIOMFAC). In addition, particle-phase behaviour, including the prevalence of liquid–liquid phase separation (LLPS), was also modelled with AIOMFAC.

By comparison with HTDMA data, it was also found that the model was capable of capturing the behaviour of different mixtures of AS/PEG/dicarboxylic acids at high RH. Therefore, experimental data could be used for models to improve the estimation of interaction parameter for PEG group (CH2OCH2) with the carboxyl group (COOH).

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4AC.18

Accelerated Chemistry in Microdroplets: Reaction of Aldehyde Functionalities in α-Pinene Secondary Organic Aerosol with a Derivatizing Agent. YAO ZHANG, Murray Johnston, *University of Delaware*

Recent studies have shown that reaction rates in microdroplets can be accelerated by several orders of magnitude over similar processes in bulk solutions (Banerjee et al., Analyst 2017, 142, 1399). In the work presented here, α-Pinene Secondary Organic Aerosol (SOA) is analyzed online using droplet assisted ionization (DAI). When the droplets contain both SOA and the Girard T (GT) reagent, fast reaction of aldehyde functionalities in the SOA with the GT reagent give products that are detected with high sensitivity. The reaction proceeds on the order of seconds in droplets, but hardly at all after an hour in bulk solution. The experimental setup to perform accelerated reaction chemistry will be described in detail, along with a discussion of reaction products and potential applications to online molecular characterization of SOA.

4AC.19

Multiphase Product Distributions for Aqueous-phase Oxidation of Water-soluble Organic Compounds in Bulk Solution and Submicron Particles. KEVIN NIHILL, Christopher Lim, James Rowe, Martin Breitenlechner, Alexander Zaytsev, Joshua L. Cox, Frank Keutsch, Jesse Kroll, *MIT*

Atmospheric aqueous-phase oxidation has been identified as a possible source of highly oxidized organic aerosol (OA) observed in the ambient atmosphere. Most laboratory experiments monitoring the oxidation of organic precursors in the aqueous phase have used bulk phase chemistry, but this may not accurately simulate partitioning or concentration conditions of fine particles in the ambient atmosphere. This is suggested by significant differences in the product distributions of experiments that compare oxidation of water-soluble organics in both the bulk and particle phases. This work serves to extend our understanding of atmospheric aqueous oxidation of water-soluble organic compounds by precisely measuring and comparing the aqueous-phase oxidation products of varying carbon-number polyols (water-soluble compounds with formula $C_nH_{2n+2}O_n$) in both the gas and aqueous phases. Through complementary measurements of oxidation products using an aerosol mass spectrometer (AMS) and two proton-transfer reaction time-of-flight mass spectrometers (high sensitivity PTR3s) – one for the gas phase, and one with a gas-phase denuder followed by a thermodesorption unit for aerosol volatilization – we seek to understand the full oxidation product distributions for a variety of polyols. In particular, a more thorough profile of gas-phase products will allow for an improved understanding of how partitioning and concentration effects in aqueous-phase oxidation impacts the chemistry of the atmosphere. Further, we can elucidate the dependence of gas-particle partitioning on the liquid water content (LWC) of the air mass, which may span many orders of magnitude in the atmosphere. This study underscores the need to reproduce atmospheric conditions in the laboratory in order to better characterize the influence of aqueous-phase oxidation on atmospheric organic chemistry.

4AC.20

Exploring the Autoxidation Mechanisms of Aromatic VOCs. RUBY MARTEN, Mao Xiao, Lukas Fischer, Bernhard Mentler, Mario Simon, Martin Heinritzi, Olga Garmash, Christopher R. Hoyle, Andrea Baccarini, Chuan Ping Lee, Houssni Lamkaddam, Imad El Haddad, Josef Dommen, Urs Baltensperger, CLOUD Collaboration, *Paul Scherrer Institute*

It has been shown that both biogenic and anthropogenic aromatic volatile organic compounds (AVOCs) present in the atmosphere are not only important reactants in formation of secondary organic aerosol and ozone, but that they also form highly oxygenated molecules (HOMs) in the gas phase, which in turn will contribute to new particle formation due to their extremely low volatility.[1,2] In urban areas, anthropogenic AVOCs are a major atmospheric component and therefore an important part of the chemistry involved. AVOCs become HOMs after addition of OH^- to the aromatic ring and a subsequent autoxidation route with multiple additions of O2, leading to a high O:C ratio. Although the oxidation mechanism involved has been studied in depth in many laboratory and theoretical experiments, the complete mechanism of autoxidation is still not clear. Furthermore, mass spectrometry data shows clear evidence of 'dimers' of aromatic HOMs formed in the gas phase, another mechanism which remains unexplained.

This work will present results from experiments, focusing on anthropogenic AVOCs, undertaken during the CLOUD 11 (2016) and CLOUD 12 (2017) campaigns at the CLOUD (Cosmics Leaving OUtdoor Droplets) chamber at CERN. Experiments were performed with toluene, naphthalene, and 1,2,4-tri-methylbenzene under varying atmospherically relevant conditions.

A proposed general mechanism of HOM formation for aromatic VOCs will be presented in order to explain the observed products of autoxidation. This mechanism will be based off of state-of-the-art theories[3,4] combined with data collected from the CLOUD campaigns. Reaction rate constants and branching ratios for the different pathways will be proposed, to capture the observed concentrations and time series of HOMs. The general mechanism of aromatic compound oxidation and the associated rates will be presented and the implication of the different pathways in the HOMs production will be discussed.

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4AC.21

PIXE Analysis of PM2.5 Atmospheric Aerosols in a Two Year Monitoring in Mexico City. VALTER ARMANDO BARRERA, Raul Venancio Diaz, Javier Miranda, Giulia Calzolai, Silvia Nava, Martina Giannoni, Franco Lucarelli, *CONACYT-CIACYT/UASLP, Mexico*

After more than 25 years of local air pollution monitoring in Mexico City, Particle Matter (PM) is one pollutant that is not decreasing. This is due to many factors, like the well-known geography, the Ozone all year production with the subsequent reactivity in the local atmosphere, and natural or anthropogenic sources; the Metropolitan Area of Mexico City (MAMC), is still growing without control (8 M inhabitants plus 12 M inhabitants in Mexico City basin). Moreover, the number of vehicles (more than 4.5 M) increases with no regulation and finally, there are industrial zones around the megacity.

Last decades, multiple elemental studies have been done for different PM fractions (Miranda et al., 1992, 1998, 2004, 2005; Chow et al., 2002; Barrera et al., 2012; Diaz et al., 2014). However, there is a lot to know of the chemical composition of the PM pollutant in Mexico city in the recent years, mainly the fine fraction or $PM_{2.5}$.

This work presents a Particle Induced X-ray Emission (PIXE) analysis and a source apportionment study of $PM_{2.5}$ in a two-year monitoring campaign, collecting samples in 4 sites to provide a wider knowledge of elemental concentrations. Monitoring sites were located at the southwest and southeast city for year 2009 and for 2010 at southwest and downtown Mexico City. Almost 200 $PM_{2.5}$ samples were collected on a 24 h (from midnight to midnight) sampling base each two days, by using two Teom samplers (medium-volume 1 m^3/h), depositing the particles onto 47 mm diameter Teflon filters, allowing the application of the PIXE technique. Meteorological parameters were obtained from the local network.

PIXE analyses were performed at the 3 MV Tandetron accelerator of the INFN-LABEC laboratory, with a recently installed external beam set-up composed by a Silicon Drift Detector with a large active area (80 mm^2) and 450 mm thickness for low Z element, with proton deflector and an identical SDD detector used just for the detection of medium-high energy X-rays, thus reducing the irradiation time and generating better statistical data (Lucarelli et al., 2014). Each sample was irradiated for ~90 s with a 3.0 MeV proton beam (~2 mm^2 spot, 10 nA to 150 nA intensity). PIXE spectra were fitted using the GUPIX code (Maxwell et al., 1995) and elemental concentrations were obtained by a calibration curve from a set of thin standards of known areal density (Micromatter Inc.). The lighter elements (Na, Mg, Al and Si) concentrations were corrected for self-absorption effects (Calzolai et al., 2010). Also, PIXE technique provide a better analysis for several trace elements that are very useful for aerosol source apportionment (e.g., V, Ni, Cu, Zn, Pb) (Maenhaut, 2015). Uncertainties were determined by a sum of independent uncertainties or an expanded uncertainty method from each analysis (Espinosa et al., 2010).

More than 20 elements were identified by PIXE, representing more than 12% of the $PM_{2.5}$ total mass in the four sites. Maximum concentrations episodes were registered in the two corresponding monitoring zones at Feb 12th, 2009 and June 1st, 2010, mainly due to different industrial zones near the MAMC.

Different multivariate methods were used to determine the number of possible influencing polluting sources for each site, which were then identified through back-trajectory simulations with the HYSPLIT modeling software (Draxler & Rolph, 2010).

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4AC.22

Vertical Characterization of Highly Oxygenated Molecules (HOM) Below and Above a Boreal Forest Canopy. QIAOZHI ZHA, Chao Yan, Heikki Junninen, Matthieu Riva, Juho Aalto, Lauriane Quéléver, Simon Schallhart, Lubna Dada, Liine Heikkinen, Otso Peräkyla, Jun Zou, Clemence Rose, Yonghong Wang, Ivan Mammarella, Timo Vesala, Douglas Worsnop, Gabriel Katul, Markku Kulmala, Tuukka Petäjä, Federico Bianchi, Mikael Ehn, *University of Helsinki*

Highly oxygenated molecules (HOM) play important roles in new particle formation (NPF) and secondary organic aerosol (SOA) formation, and therefore have significant effect on air quality, global radiation budget, and climate. In addition to the efforts that have been made in understanding the formation mechanisms of HOMs, increased attention has been drawn to the interaction between HOM chemistry and changing atmospheric conditions.

During the Influence of Biosphere-Atmosphere Interactions on the Reactive Nitrogen budget (IBAIRN) campaign, vertical profile measurements of HOMs below and above the forest canopy were performed using two nitrate ion based Chemical Ionization Atmospheric Pressure interface Time-Of-Flight (CI-APi-TOF) mass spectrometers, for the first time in the boreal forest SMEAR II station during September 2016. The HOM concentrations and composition distributions below and above the canopy were similar in the well-mixed boundary layer condition during daytime. Surprisingly, during night, even though precursor monoterpene concentrations are elevated, much lower HOM concentrations were observed at ground level, as a result of the formation of a shallow decoupled layer attached to the forest floor. The results suggested that near ground HOMs were affected by the changes in the precursors and oxidants, and enhancement of the loss/deposition on surfaces in this layer, while the HOMs above the canopy top were not significantly affected.

One of the main novelties of our study is the detailed measurements of HOM below and above the canopy across a wide range of atmospheric stability conditions. The results highlight the significance of near-ground boundary layer dynamics and micrometeorological processes to the ambient HOMs, and the ground-based HOM measurement are not always representative for the entire boundary layer. This needs to be considered when interpreting measurements that are expected to be influenced by HOM, such as growth rates of new particles.

4AC.23

Fine Particle pH in Urban Guangzhou, a Megacity of South China. ZHISHENG ZHANG, Jun Tao, Leiming Zhang, Zejian Lin, *South China Institute of Environmental Sciences*

Particle acidity is a critical parameter affecting aerosol processes and properties, yet it is poorly constrained in China. In the present study, hourly measurement of particulate and gaseous compositions along with meteorological parameters were observed in an urban site of Guangzhou, a megacity of South China. A total of 4688 sets of data were obtained. These data were used as inputs into ISORROPIA-Ⅱ thermodynamic equilibrium model running in the forward mode to estimate the fine particle pH. Fine particle pH in Guangzhou ranged from 1.3 to 5.7, with a mean of 2.8. It showed a clear diurnal pattern with peak value in the early morning hours and lowest value occurred in the afternoon. Higher fine particle pH were found on polluted cases when the particulate compositions were dominated by nitrate and ammonium. Sensitivity tests were performed by altering inputs to analyze the potential impacts of these variables on particle pH. It showed that NH_3, SO_4, relative humidity (RH) and temperature were the key factors affecting pH in Guangzhou. Under high RH and low temperature conditions, high NH_3 and low sulfate concentrations tended to generate high pH particles.

4AC.24

The Presence of Phenanthrene Oxidation Products in α-Pinene Secondary Organic Aerosol Particles. AMBER KRAMER, Kaitlyn J. Suski, Alla Zelenyuk, Staci L. Simonich, *Oregon State University*

Polycyclic aromatic hydrocarbons (PAHs) are toxic environmental pollutants which are transported globally on fine particulate matter (PM2.5) and monitored in many parts of the world. Phenanthrene is a ubiquitous model three-ringed PAH. Secondary organic aerosols (SOA) are naturally formed through atmospheric reactions of biogenic volatile organic compounds, making up a large fraction of PM2.5, and have been shown to trap and transport PAHs. SOA particles have been shown to consist of highly oxidized organic compounds and reactive oxygen species, which have the potential to react with other organic components such as PAHs, changing the physical properties of the particles and their ability to enhance long range atmospheric transport. The presence of oxidized PAHs has been shown, and needs to be explored to improve atmospheric transport modeling and human risk assessment. In controlled laboratory experiments, ozone reacted α-pinene SOA will be grown with gas phase phenanthrene present. Particles will be monitored for physical characteristics over time, and filters of SOA particles will be collected and analyzed for phenanthrene and phenanthrene oxidation products. Collected SOA filters will be extracted and analyzed using gas-chromatography partnered with mass spectrometry to determine the chemical makeup of the phenanthrene within the particles. The specific compound mixtures will be screened for changes in oxidative potential and developmental toxicity. Preliminary experiments have shown that PHE reacts within SOA system to form mono-hydroxy PHE, and poly-hydroxy PHE compounds. Data also shows that the ratios of compounds continues to change over aging of the particles, and with exposure to ozone.

4AC.25

Clustering of Sulfuric Acid, Bisulfate Ion and Organonitrate C10H15O10N: Thermodynamics and Atmospheric Implications. JASON HERB, Alexey Nadykto, Kirill Nazarenko, Nikolai Korobov, Fangqun Yu, *SUNY at Albany*

Recently, Highly Oxidized Molecules (HOMs) have been suggested to play an important role in New Particle Formation (NPF) in the atmosphere. Although stable clusters containing organonitrates (ONs), a common form of HOM containing nitrogen in addition to carbon, hydrogen and oxygen, and neutral and negatively charged sulfuric acid molecules have been detected in both laboratory experiments under atmospherically relevant conditions and in-situ measurements, the role of ONs in their stability is still poorly understood. In this study, we seek to advance the understanding of the role of ONs in atmospheric NPF by carrying out a Density Functional Theory (DFT) study of the bonding of a selected $C_{10}H_{15}O_{10}N$ organonitrate, N-[2-(1,2-Dicarboxyethoxy)ethyl]-3-hydroxyaspartic acid with H_2SO_4 and bisulfate ion HSO_4^-. The present analysis reveals an important role of the $C_{10}H_{15}O_{10}N$ in the enhanced stability of both ionic and neutral clusters as all the mixed dimers, trimers and tetramers containing $C_{10}H_{15}O_{10}N$ are found to be more stable compared to pure ones. The substitution of the H_2SO_4 molecule with the ON is particularly favorable in the case of negative ions, when the stepwise Gibbs free energy increases by up to ~9 kcal mol^{-1} per step due to the presence of the ON. In particular, the free energies of the formation of $(H_2SO_4)_{n-1}(ON)(HSO_4^-)$ and $(H_2SO_4)n(HSO_4^-)$ via the addition of H_2SO_4 differ by 0.7, 5.45 and 9.2 kcal mol^{-1} at n=2, 3 and 4, respectively, in the favor of $(H2SO4)_{n-1}(ON)(HSO_4^-)$ clusters. The effect of the $C_{10}H_{15}O_{10}N$ on clustering of H_2SO_4 molecules under is smaller, but still considerable as evidenced by ~ 0.7-2 kcal mol^{-1} difference in the formation free energies, also in the favor of ON-containing clusters. This indicates that the $C_{10}H_{15}O_{10}N$ is capable of facilitating the production of fairly large sulfuric acid clusters and may promote in this way atmospheric NPF under favorable conditions.

4AC.26

SOA Formation from Toluene Oxidation in the Presence of Nox: The Importance of Relative Humidity. DAO HUANG, Yunle Chen, Masayuki Takeuchi, Taekyu Joo, Steve Kim, Gamze Eris, Nga Lee Ng, *Zhejiang University*

Toluene is one of the most important anthropogenic volatile organic compounds (VOCs) considering its high concentration in urban and some rural areas and high secondary organic aerosol (SOA) yields. However, in the past decade, knowledge about toluene SOA in the presence of NOx is limited to SOA yield curve under dry conditions and a few scattered yields under humid conditions. Little is known about toluene SOA composition and the effects of relative humidity (RH) on toluene SOA yields and composition. In the present work, a series of toluene photooxidation experiments under dry and humid conditions were performed in the Georgia Tech Environmental Chamber facility (GTEC) to investigate the toluene SOA composition and RH effects. In situ photolysis of HONO was used as an OH radical and NOx sources. Ammonium sulfate was used as aerosol seeds. Particles were chemically characterized using a high-resolution time-of- flight aerosol mass spectrometer (HR-ToF-AMS) and a high-resolution chemical ionization time-of-flight mass spectrometer coupled with a filter inlet for gas and aerosol (FIGAERO-CIMS). Simultaneously, gas-phase compounds were determined by CIMS. Based on experimental results, we obtain different SOA yield curves as a function of organic aerosol (ΔMo) at various RH and compare the particle composition under dry and humid conditions. Generally, the molecular weights of SOA compounds generated under humid conditions is much smaller than that under dry conditions. Under humid conditions, oxygenated organic compounds containing 6 or fewer carbons are the major components of SOA. Under dry conditions, organic nitrates containing 7 or more carbons are the main components of SOA. Further, the evolution of SOA composition over time is also different under dry and humid conditions. We also investigate SOA formation mechanisms under humid conditions by comparing experimental results with MCM modeling. Studying toluene SOA composition and the role of water in SOA formation is important for understanding SOA and haze formation in the real atmosphere.

4AC.27

Modeling the Impact of Cookstove Emissions on Ambient Aerosol in Rural India. BRIGITTE ROONEY, Kirk Smith, John Seinfeld, Ajay Pillarisetti, Rufus Edwards, Lauren Fleming, Sergey Nizkorodov, Tami Bond, Nicholas Lam, Sumit Sharma, Seema Kundu, Shaocai Yu, Pengfei Li, Kelvin Bates, Ran Zhao, *California Institute of Technology*

In India, particulate matter (PM) pollution is a significant cause of health problems and increased mortality. However, specific source contributions to PM have remained largely understudied, as work that has been done has mostly focused on indoor air quality. Within the residential sector, a majority of Indian households still rely on solid biofuels, mainly wood and dung, for cooking. Combustion of solid fuels is known to produce more aerosol than liquid fuels, and thus cookstove use has been identified as a potential significant source of PM pollution.

To better understand the production of ambient aerosol by the residential sector in rural India, we have undertaken a series of modeling experiments using the Community Multiscale Air Quality (CMAQ) atmospheric chemistry transport model. This work incorporates updated emissions inventories and time varying boundary conditions, and represents some of the highest resolution (1km and 4km grid cells) modeling of its kind. By varying such parameters as fuel type and emission factors, we are able to determine the fraction of PM attributable to cookstove use. Our expectation is that the results will further incentivize the transition from household use of solid fuels to more modern liquid fuels in order to reduce the health risks associated with aerosol pollution.

4AC.28

A Laboratory and Modeling Investigation on the Effects of Ammonia Uptake on SOA Composition and Its Potential Impacts on Air Quality.

JULIA MONTOYA-AGUILERA, Mallory Hinks, Jeremy Horne, Shupeng Zhu, Donald Dabdub, Sergey Nizkorodov, *University of California, Irvine*

Particulate matter (PM) consists of suspended particles in the atmosphere large enough to diminish visibility, affect global temperatures by absorbing or scattering light, and contribute to cloud formation by acting as cloud condensation nuclei (CCN). The importance of inorganic nitrogen contribution to PM is well recognized and included in air quality models. Less understood is the contribution of nitrogen-containing organic compounds (NOC) to secondary organic aerosols (SOA), a major component of PM. Currently, the reactive uptake of ammonia (NH_3) leading to the formation of NOC in SOA remains unaccounted for in air quality models. Ammonia is ubiquitous in the atmosphere and is emitted largely from agricultural processes. Intensifying use of NH_3-based fertilizers suggest NH_3 levels will continue to rise in the future. It is important to better characterize this NH_3 uptake process, not only because of its potential effects on SOA composition, but also because, if the uptake is efficient, NH_3 may be unavailable to contribute to inorganic PM formation.

This study investigates the effects of NH_3 on SOA formation, optical properties, and chemical composition. Anthropogenic (toluene, n-hexadecane) and biogenic (isoprene, limonene) volatile organic compounds (VOCs) are oxidized in a smog chamber at various relative humidity and NO_x levels. After SOA formation, a pulse of gas-phase NH_3 is introduced into the chamber. Particle growth is monitored with a scanning mobility particle sizer (SMPS). A proton-transfer-reaction time-of-flight mass spectrometer (PTR-ToF-MS) is used to track VOCs. An NH_3 analyzer is used to measure the decay of ammonia onto particles (and chamber walls) and a time-of-flight aerosol mass spectrometer (ToF-AMS) is employed to monitor the increase in N:C ratios in the organic components as well as increases in ammonium ion in the aerosol particles. Subsequently, samples are collected and analyzed via direct analysis in real time mass spectrometry (DART-MS). These techniques are used to determine to what extent NH_3 reacts with SOA to form NOC (as opposed to being neutralized to ammonium ions by organic and inorganic acid vapors). Additionally, wavelength dependent mass absorption coefficients of SOA extracts are measured. Results indicate that the rate and maximal extent of the NH_3+SOA→NOC reactions vary depending on the SOA system. Of the SOA studied, limonene SOA was the most reactive when exposed to NH_3. DART mass spectra revealed that exposure of limonene SOA to NH_3 converted up to 20% of SOA compounds to NOC. The experimental results were incorporated into the University of California, Irvine - California Institute of Technology (UCI-CIT) model, a state-of-the-art airshed model used to evaluate air quality in the South Coast Air Basin of California (SoCAB). A surface reaction of NH_3 with SOA was implemented into the model to estimate the impact on NH_3 and $PM_{2.5}$ concentrations in the SoCAB region. Results indicate the chemical uptake of NH_3 by SOA can potentially deplete gaseous NH_3 concentrations, leading to indirect reductions in the amount of ammonium nitrate and ammonium sulfate in PM. Moreover, the impact of this chemical uptake was investigated on a larger scale by incorporating the results into the Community Multiscale Air Quality Modeling System (CMAQ) model, with a domain covering the continental United States. The CMAQ model simulations show that inclusion of the NH_3+SOA→NOC chemistry decreases the concentration of inorganic components of $PM_{2.5}$ but increases biogenic SOA, especially in the southeastern United States.

4AC.29

Secondary Organic Aerosol Production from Healthy and Aphid-Stressed Scots Pine Biogenic Volatile Organic Compound Emissions in Different Oxidant Systems. FATEMEH KHALAJ, Celia Faiola, Angela Buchholz, Eetu Kari, Arttu Ylisirniö, Minna Kivimäenpää, Jarmo Holopainen, Annele Virtanen, *University of California, Irvine*

Vegetation emits copious amount of hydrocarbon compounds into the atmosphere, called biogenic volatile organic compounds (BVOCs). BVOCs amount to about 90% of global total VOC emissions. Most BVOCs, based on their high reactivity, have short life times (a few hours), and readily react with atmospheric oxidants to produce lower volatility oxidation products. Thus, BVOCs are major precursors of atmospheric secondary organic aerosols (SOA). Biotic stressors, such as increased insect herbivory, enhance BVOC emissions and modify the types of BVOCs emitted. For example, methyl salicylate (MeSA) is a plant hormone induced by aphid herbivory. However, it is unclear how plant stress emissions such as MeSA alter SOA production. In this study, healthy and aphid-stressed Scot Pine BVOC emissions were used to evaluate SOA production during oxidation via ozonolysis or photooxidation. SOA was generated in Kuopio, Finland a 10 m3 batch reaction chamber composed of FEP material. For comparison to the healthy and stressed Scots pine experiments, SOA was generated from single component standards, α-pinene (OH and O3), and MeSA (OH only). For the plant SOA experiments, Scots pine saplings were enclosed in a dynamic enclosure with flow rates ~4 lpm, their emissions were trapped onto adsorbent cartridges overnight, and then thermally desorbed into the batch reaction chamber targeting ~20 ppb initial monoterpene mixing ratios at the start of the experiment. The initial suite of BVOCs that acted as SOA precursors during the Scots pine experiments was characterized via thermo-desorption gas chromatography mass spectrometry (TD-GC-MS). BVOC concentrations were monitored continuously throughout oxidation with a high resolution proton transfer reaction mass spectrometer (PTR-ToF-MS; Ionicon, Inc.). Particle size distributions and composition were monitored with a scanning mobility particle sizer (SMPS; TSI, Inc.) and high resolution time of flight aerosol mass spectrometer (HR-ToF-AMS), respectively. Results of BVOC concentrations demonstrated that aphid herbivory led to higher mixing ratios of sesquiterpenes in the reaction chamber. The average sesquiterpene mixing ratio was 1.84±1.12 ppb and 8.74±0.04 ppb for healthy and stressed Scots pine experiments, respectively. For comparison, the average monoterpene mixing ratio was 21.68±4.44 ppb and 22.60±1.36 ppb for healthy and stressed Scots pine experiments, respectively. The average MeSA mixing ratio was 1.23±1.05 ppb and 0.97±0.02 ppb for healthy and stressed Scots pine experiments, respectively. The detailed molecular speciation of initial BVOC composition will be presented. Additionally, an overview of SOA mass yields and composition will be shown to compare between healthy and stressed Scots pine SOA and the two single component standards for the two oxidant systems studied.

4AC.30

Characteristics of PM2.5 and Gaseous Precursor in Urban and Background Areas in Korea. TAEHYUN PARK, Jihee Ban, Seokwon Kang, Gyutae Park, Kyunghoon Kim, Min Seok Song, Seung Hwan Lee, Jannatul Maoa, Hye Jung Shin, Jong Sung Park, Seung Myung Park, Jun Oh, Mindo Lee, Sang-Bo Lee, Jeong Soo Kim, Dong-Gil Yu, Taehyoung Lee, *Hankuk University of Foreign Studies, Yongin, South Korea*

The Korean peninsula is a great place to study different sources of the aerosols: urban, rural and marine. In addition, Seoul is one of the large metropolitan areas in the world and has a variety of sources because half of the Korean population lives in Seoul, which comprises only 12% of the country's area. Also, Baengnyeong island located in the west of Korean peninsula is an important place where we can observe the behavior of air pollutants emitted from Northeast Asia and measure the background concentrations of air quality in Korea. To understand the chemical composition of aerosol from long-range transport and local sources better, both particulate matter and gaseous precursors need to observation. In this study, we plan to measure the chemical compositions of $PM_{2.5}$ (Na^+, NH_4^+, K^+, Mg^{2+}, Ca^{2+}, SO_4^{2-}, NO_3^-, Cl^-, WSOC) and gaseous precursors (HNO_3, NH_3, SO_2) by AIM(Aerosol Ion Monitor, URG Corporation), PILS(Particle Into Liquid Sampler) coupled with TOC (Total Organic Carbon, SIEVERS 850) and gas monitors (SO_2 (43C, Thermo Scientific), NH_3 (EAA 911-0016, Los Gatos Research)) in the Seoul and Baengnyeong island Intensive Air Quality Monitoring Stations during the two time of intensive period (Jan. 15 – Feb. 10, 2018 and March, 2018). The AIM and PILS-TOC is providing the ionic chemical compositions of $PM_{2.5}$ and the concentrations of gaseous precursors and water soluble organic carbon with 1-hour time resolution. The scientific goal of this study is to characterize chemical properties of $PM_{2.5}$ and gaseous precursors to understand the role of the long-range transport from northeast Asia and influence of the local sources. The presentation will provide an overview of the ionic compounds of $PM_{2.5}$ and gaseous precursors in the air pollution plume at Seoul (urban site) and Baengnyeong island (background site).

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4AC.31

Reactions between SO_2 and Organic Peroxides and Their Role as Atmospheric Sinks of Sulfur. SHUNYAO WANG, Shouming Zhou, Ye Tao, Jianhuai Ye, Jian Zhen Yu, Jennifer G. Murphy, Jonathan Abbatt, Arthur W. H. Chan, *University of Toronto*

While SO_2 oxidation has long been recognized as a source of particulate sulfate and acid rain, the underlying mechanisms by which SO_2 reacts with multiple organic species remain poorly understood. Previous chamber studies have shown that organic peroxides from monoterpene ozonolysis can react with SO_2, suggesting that organic peroxides (ROOR or ROOH) could be an important sink of SO_2. In this work, we investigate the kinetics and mechanisms of reactions between SO_2 and organic peroxides. Upon SO_2 exposure in a bulk solution, the depletion of both ROOR and ROOH standards (including cumene hydroperoxide, tert-butyl hydroperoxide, 2-butanone peroxide, benzoyl peroxide and tert-butyl peroxide) was monitored using iodometric-spectrophotometric method and was found to be significant. The reaction rate constant will be derived from the decay of total S (IV) concentration (monitored by ion chromatography) and speciated organic peroxide concentration (monitored by atmospheric pressure chemical ionization tandem mass spectrometry). In addition to the formation of inorganic sulfate, organosulfates (OS) were also formed, and were quantified by electrospray ionization ion mobility mass spectrometry (ESI-IMS) under negative mode with collision induced dissociation, using both synthetic biogenic OS and commercial OS as calibration standards. In addition to bulk solution studies, we also conduct flow tube experiments to study the reactive uptake coefficients (γeff) for SO_2 and biogenic SOA (i.e. α-pinene, isoprene). Measured kinetic parameters can be further applied to the atmospheric models to assess the potential impacts. Our work will improve understanding of how the interaction between SO_2 and organic peroxides will influence the formation of biogenic SOA under atmospheric-relevant conditions.

4AC.32

The Effect of Chemistry and Particle Total Surface Area on Loss Rate of Highly Oxidized Multifunctional Organic Molecules (HOMs).

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The loss of Highly Oxidized Multifunctional Organic Molecule (HOM) peroxy radicals on existing particle surface as reported here might have implications on atmospheric chemistry. Particle densities used in the experiments correspond to mass loadings observed in the Troposphere. HOM-RO_2 lifetimes in the atmosphere are also likely to be longer than in our experiments, leading to proportionally higher importance of condensational loss onto particles.

HOMs are a group of organic molecules produced by oxidation of VOC, and are generally considered to have low to extremely low vapour pressures, which makes them potentially important in particle formation and growth processes in the atmosphere. Better understanding the formation and loss processes of these molecules can thus lead to a better understanding of particle formation.

HOM formation can be explained by peroxy radical chemistry: a HOM peroxy radical (HOM-RO_2) is formed via autoxidation, followed by a termination via classical peroxy radical pathways. The main stable end product pathways are those leading to formation of ketones or alcohols (RO_2+RO_2’), and hydroperoxides (RO_2+HO_2).

When studying the formation and loss processes of HOMs in chamber experiments we discovered that there were indications that the particles were participating photochemistry, in that they acted as a condensation sink to both HO_2 and HOM-RO_2. This was observed during determinations of effective uptake coefficients of HOM on particles. For HOM with extremely low vapour pressures uptake coefficients are 1, i.e. uptake by particles is collision limited. At high particle surface ($> 1.0 \cdot 10^{-3}$ m^2m^{-3}), uptake coefficients for some HOM seemed to be higher than 1, while for other HOM loss rates decreased with increasing particle surface. Our hypothesis is that also peroxy radicals are lost on particles. When in presence of high particle surface, losses of peroxy radicals on particles affect the production rates of termination products. Lower production rates mimic too high uptake coefficients and vice versa higher production rates can mimic decreases of uptake coefficients at higher particle surface.

Examples for this behaviour are the HOM dimers. Lower peroxy radical concentrations due to efficient losses on particles decrease production rates and pretend uptake coefficients higher than collision limited. Another observation indirectly indicates very efficient HO_2 losses on organic particles. HOMs preliminary identified as hydroperoxides show the same behaviour as dimers and other HOM preliminary identified as ketones show the opposite trend. We suggest that the HO_2 losses lead to lower production rates of hydroperoxides with the result of unrealistically high uptake coefficients. The apparent lowering of uptake coefficients for ketones suggests that the HO_2 losses can also lead to an increasing production rate in RO_2+RO_2 reactions.

4AC.33

Secondary Organic Aerosol Formation from Methylfurans by Nitrate Radical Oxidation. TAEKYU JOO, Masayuki Takeuchi, Matthew Alvarado, Nga Lee Ng, *Georgia Institute of Technology*

An important activity that contributes to both primary organic aerosol (POA) and secondary organic aerosol (SOA) formation is biomass burning. Recent studies about biomass burning SOA formation demonstrate that a large fraction of SOA is produced from an unidentified pathway. These studies suggest an important contribution of nontraditional precursors to SOA formation from biomass burning, such as furan derivatives. Methylfurans are one of the main furan derivatives that are emitted by biomass burning. However, our current understanding of SOA formation from methylfurans is extremely limited, and even less attention has been paid to nighttime oxidation of this class of compounds from biomass burning activities. Here, we investigate SOA formation from 2- and 3-methylfuran by nitrate radical (NO_3) oxidation at the Georgia Tech Environmental Chamber (GTEC) facility. NO_3 is formed from NO_2 + O_3 reaction, and NO_3 subsequently reacts with NO_2 to make N_2O_5. The VOC:N_2O_5 ratio was set around 1:4 to ensure peroxy radicals react with NO_3. Oxidation products were measured in real-time with High Resolution Time-of-Flight Chemical Ionization Mass Spectrometer (HR-ToF-CIMS) coupled with a Filter Inlet for Gases and AEROsols (FIGAERO). This setup allows the measurement of both gas- and particle-phase composition during the oxidation process. A High Resolution-Time of Flight-Aerosol Mass Spectrometer (HR-ToF-AMS) was deployed to measure the bulk elemental composition of SOA. The VOC decay was measured with Gas Chromatography Flame Ionization Detector (GC-FID) and the increase of aerosol mass concentration was measured with a Scanning Mobility Particle Sizer (SMPS). Aerosol mass continued to increase after all 2- and 3-methylfuran were consumed, indicating a large contribution of higher-generation oxidation products to SOA. Organic nitrate ($RONO_2$) contribution was around 10-15% to the total organics measured by HR-ToF-AMS. Multiple monomer and dimer species that contain an -ONO_2 functional group were also detected by FIGAERO-ToF-CIMS. These results indicate that the $RONO_2$ species are also important in terms of SOA formation, which have not yet been considered in 2- and 3-methylfuran SOA studies to date.

4AC.34

Soil Spreading of Organic Waste Products: Source of Secondary Oorganic Aerosols. RALUCA CIURARU, Corentin Berger, Pauline Buysse, Yvain Carpentier, Céline Decuq, Cristian Focsa, Sophie Genermont, Sylvie Gosselin, Sabine Houot, Julien Kammer, Florence Lafouge, Benjamin Loubet, Nicolas Visez, Denis Petitprez, *INRA*

The agricultural soils emit volatile organic compounds (VOCs) that contribute to the formation of secondary pollutants such as ozone or secondary organic aerosols (SOA).

Soil VOC emissions are lower than the VOCs released from the canopy. Nevertheless, it has been showed that under certain conditions (i.e., temperature, soil water content…) and for specific ecosystems, VOC emissions from soil could reach the same order of magnitude as canopy emissions (Peñuelas et al., 2014). Data on VOC released from agricultural soils are relatively scarce although they are recognized as large contributors of methanol and acetone to the atmosphere (Bachy et al., 2018).

Organic waste products (OWPs) are used in agriculture as organic amendments to improve soil fertility. The valorization of different types of OWPs from farms (bovine manure, pig slurry…), urban origin (sewage sludge, green waste) or industrial origin (sweets, etc.) is currently promoted as a substitute for mineral fertilizers. OWPs have a wide variety of characteristics due to their origin and the treatments that they may undergo before spreading and this diversity of characteristics could have a significant impact on gaseous and particulate emissions following soil application. There are few studies quantifying the concentrations and emission rates of gaseous compounds emitted from organic waste products, and those studies primarily address their odorant properties in order to identify suitable odor abatement techniques (Feilberg et al., 2015). Some of these laboratory studies have quantified the VOCs emissions from OWPs, including non-methane hydrocarbons VOCs, sulfur compounds, nitrogen compounds and oxygenated volatile organic compounds (Feilberg et al., 2015). Chemical transformations of these atmospheric organic compounds can further lead to products of lower volatility that subsequently partition into the condensed phase.

The aim of this study is to investigate VOC emissions, their subsequent reaction with ozone and SOA formation from agricultural soil amended with different OWPs. The experiments are currently performed in an atmospheric chamber coupled to an aerosol flow tube. A high panel of scientific equipment allows the physical and chemical characterization of the VOCs and freshly formed aerosols (proton transfer mass spectrometer, scanning mobility particle sizer…). Aerosol sampling on filters allows their chemical and molecular characterization by off-line analysis (gas chromatography, time of flight secondary ions mass spectrometry, laser desorption/ionization time of flight mass spectrometry).

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4AC.35

PRAPPE: Trace Element Interaction with Organic Compounds in Urban and Crustal PM. JOSEPH SALAZAR, David Pfotenhauer, Frank Leresche, Fernando Rosario-Ortiz, Michael Hannigan, Brian Majestic, *University of Denver*

As part of a larger study, we present field data from the Platte River Air Pollution and Photochemistry Experiment (PRAPPE), aimed at understanding the interactions between organic carbon and trace elements in atmospheric particulate matter (PM). One transformation pathway of organics in the atmosphere is radical oxidation. One possibly unexplored route of radical formation is iron in aqueous suspension via the Photo-Fenton reaction. In Fenton Chemistry, UV light reacts with iron (III) to produce iron (II) and hydroxyl radicals. In turn, the hydroxyl radicals oxidize organic compounds. In this portion of the study, we investigate the role of metals in this process by collecting simultaneous PM2.5 samples in three regions: urban, rural, and a mixture between the two. Sampling was accomplished during the summer (Aug. 2017) and winter (Dec. 2016 - Mar. 2017), where 24-hr PM2.5 samples were collected at three different sites on the Eastern Colorado plains. At each site, three filters were collected: two Teflons (mass, ions, soluble metals, and total metals) and 1 quartz filter (EC/OC and organic speciation). Part of the Teflon filter was also analyzed by x-ray absorption near edge structure (XANES) spectroscopy to probe the oxidation state of iron in the PM. Understanding the oxidation state of the iron is an important factor in determining its solubility, where Fe(II) tends to be the more soluble of the iron species, and thus would be most important in radical production. In addition, XRF maps of each sample were collected to understand intraparticle composition. During the winter, the urban and mix site showed the same levels of iron concentration (average = 2.70 ng/m^3) while the crustal site showed significantly less iron (average = 0.78 ng/m^3). This is one of two abstracts for this project. Here, we work to quantify and understand the state of iron in the different sources of PM while another abstract will present data on the influence of iron on the formation of hydroxyl radical upon photoirradiation of aqueous PM extracts and on the effect of irradiation on the light absorbance properties and hydroxyl radical formation potential of the extracts. These results will be the first attempt in the understanding how iron processes organic compounds through reactive oxygen species in PM collected from urban and rural sources.

4AC.36

Analysis of Gas-phase and Particulate Reaction Products from High-NOx Photooxidation of n-dodecane: Influence of Temperature and Relative Humidity on Secondary Organic Aerosol Formation. HOUSSNI LAMKADDAM, Aline Gratien, Edouard Pangui, Mathieu Cazaunau, Marc David, Jean-Michel Polienor, Murielle Jerome, Cécile Gaimoz, Bénédicte Picquet-Varrault, Jean-François Doussin, *LISA, Universités Paris-Est-Créteil et Paris Diderot*

Organic aerosol (OA) plays an important role on atmospheric chemistry, climate change and public health. While OA particles can be directly emitted into the atmosphere, they can also be introduced in the atmosphere by secondary organic aerosol (SOA) formation. However our current knowledge of oxidation pathways and chemical composition of the SOA is limited and poorly understood considering the difficulty of the chemical transport model (CTM) to predict the OA mass in the atmosphere (Heald et al., 2011). It results to large uncertainties in the estimation of the impact on climate and air quality of the atmospheric aerosols.

In this context, the aim of this work is to study SOA formation from oxidation of precursors such as long chain alkanes which represent a substantial fraction of the unresolved complex mixture in diesel fuel (Gentner et al, 2012). Beside the fact that it represents a relevant class of compound for the urban atmosphere, long chain alkanes are also very interesting model-molecule to investigate the sensitivity to different reaction pathways of the organic matter, i.e. fragmentation, functionalization or oligomerization, during its atmospheric oxidation.

The experiments were carried out in the CESAM chamber (http://cesam.cnrs.fr) (Wang et al., 2011). It is a 4,2 m3 stainless steel chamber which allows to conduct experiments at different temperature and relative humidity, constant pressure and under a very realistic actinic flux. It is also equipped with a large range of analytical instruments to characterize the gas-phase and particulate reaction products.

In particular, the present work assesses the effect of temperature (from 10 to 30°C) and relative humidity (from <1 to 70%) on the high-NOx photooxidation of n-dodecane. Aside aerosol mass production, the mechanism was also investigated by measuring SOA composition. Mechanistic pathways of the gaseous and particulate products will be proposed.

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4AC.38

Reactions between Small Atmospheric Carbonyls and Ammonium Sulfate. MELISSA GALLOWAY, Daisy Grace, Melissa Sebold, Rachael Holappa, Jessica Ackendorf, *Lafayette College*

The chemical composition of atmospheric aerosol is complex and poorly understood. Aqueous reactions of aldehydes with amines or ammonium salts have been implicated in atmospheric brown carbon formation processes. Recent work has started to identify the products of these reactions, especially those responsible for visible light absorbance. However, few studies have looked at the reaction products of ammonium with a mixture of aldehydes. Supercritical fluid chromatography-electrospray ionization-mass spectrometry equipped with a photodiode array is tested as a viable technique for separation and identification of the reaction products of mixtures of small, water soluble carbonyls (e.g. glyoxal, methylglyoxal, and glycolaldehyde) with ammonium sulfate. We present information on the efficacy of this separation technique as well as structural and mass comparisons between products formed from the reaction of a single aldehyde with ammonium and a mixture of aldehydes and ammonium sulfate. The results of these studies will allow us to better understand the aqueous chemistry occurring in atmospheric aerosol droplets.

4AC.39

Molecular Insights from Ultrahigh Resolution Orbitrap Mass Spectrometry on Aqueous Phase Processing of Ambient Biomass Burning Emissions Influenced Po Valley Fog and Aerosol. MATTHEW BREGE, Tyler Leverton, Stefania Gilardoni, Stefano Decesari, Marco Paglione, M. Cristina Facchini, Lynn Mazzoleni, *Michigan Technological University*

Ambient samples of fog water and PM_1 aerosol were collected in the Po Valley (Italy) over four consecutive days in the winter of 2015. The Po Valley has an established history of regional biomass burning emissions influence and aqueous aging processes resulting in significant concentrations of brown carbon. Four samples of fog water and eight samples of extracted PM_1 aerosol filters (day and night samples) were analyzed by ultrahigh resolution Orbitrap mass spectrometry using both electrospray ionization and atmospheric pressure photoionization methods. The water-soluble organic matter of the samples was fractionated prior to analysis using a 2-step solid phase extraction procedure for HULIS. This fractionation method facilitated the observation of additional less easily ionized condensed aromatic species. Thousands of distinct molecular formulas were assigned to the monoisotopic masses of each sample, and were categorized into elemental groups and sub-classes based on the observed number of oxygen, nitrogen and/or sulfur atoms in the formulas. An atypically large frequency of molecular formulas containing nitrogen and sulfur were observed. Many of which could be attributed to multifunctional organonitrates and organosulfates, however aromatic species with lower numbers of oxygen abundant in atmospheric pressure photoionization could not. In general, higher numbers of CHNO species were observed in aerosol samples and higher numbers of CHOS species were found in fog water. The observed molecular trends were related to the atmospheric conditions to determine their likely origins. The overlapping collection time periods between the two sample types, and the progressive chronological sampling, allowed for a unique perspective on chemical transformations within this humid atmosphere.

4AC.41

Effect of Aqueous-Phase Processing on Formation and Evaluation of the Organic Aerosol during Fog Processing in Kanpur, India. ANIL KUMAR MANDARIYA, Tarun Gupta, S.N. Tripathi, *Indian Institute of Technology Kanpur*

Kanpur is a polluted urban location in India, situated at the center of Indo-Gangetic Plain which witnesses several fog episodes every year during winter time and these fog episodes are linked to the enhanced in the production of secondary organic aerosol (SOA) via aqueous-phase processing. This study highlights the aqueous-phase processing of organic aerosol (OA) and relative importance of OA factors during the processing periods of fog in heavily polluted site affected by biomass emissions in the winter time. Our results show that loading of OA and inorganic species (NO_3^-, SO_4^{2-}, NH_4^+, and Cl^-) changes drastically from period of Pre-Fog-Haze to Fog and Fog to Post-Fog-Haze as compare to period of Pre-Fog to Pre-Fog-Haze and Post-Fog-Haze to Post-Fog during fog processing while mass fractions remain approximately steady, indicating the wet removal through fog droplets. Vankrevelen slopes vary throughout the periods of fog processing indicating different aging mechanism during different stages of fog processing. In contrast of aqueous phase processing mass of more oxidized oxygenated organic aerosol (MO-OOA) slightly varies throughout the fog processing periods which indicate that aqueous-phase processing plays a minor role in the formation of it as it shows poor correlation (R=0.23) with aerosol liquid water content (ALWC). In addition, fog processing has dominant impact on the formation of Low oxidized OOA (LO-OOA), oxidized biomass burning OA (O-BBOA) and biomass burning OA (BBOA) and their contribution to OA varies substantially as a function of fog periods as indicated by good significant ($p<0.05$) correlation (R=0.66, 0.66 & 0.59 respectively) with ALWC and typical fragments ions i.e. $C_2H_2O_2^+$, $C_2O_2^+$, $CH_2O_2^+$ (typical fragment ions of methylglyoxal and glyoxal) and CH_3SO^+, $CH_2SO_2^+$, $CH_3SO_2^+$ (fragment ions of methanesulfonic acid (MSA)). These results also highlighting the wet scavenging of LO-OOA, O-BBOA, and BBOA more efficiently through fog droplets as these OA components decrease significantly during the period of fog through the fog processing as compare to MO-OOA. In addition, oxygen to carbon ratio (O/C) of OA and secondary organic aerosol (SOA) also varies during the periods of fog with the maximum during Pre-Fog and Post-Fog periods as compare to rest of periods while O/C is higher during a period of Fog as compare to Pre-Fog-Haze and Post-Fog-Haze.

4AC.42

Gas-Particle Partitioning of the Traffic-Emitted Semi-Volatile Organic Compounds Measured in Fort McHenry Road Tunnel.

CHIRANJIVI BHATTARAI, Andrey Khlystov, *Desert Research Institute*

The volatility of ambient organic aerosol compounds is essential to understanding their contribution to ambient particulate matter (PM) concentrations, their atmospheric lifetime, and their effect on human health. Only recently it has been realized that primary organic aerosols (POA), such as those emitted by vehicular traffic, contain a large fraction of semivolatile substances. Data on volatility of individual semi-volatile compounds emitted by traffic is still scarce. We have sampled gas and particles phase semi-volatile organic compounds (SVOC) using Teflon-impregnated glass fiber filters (TIGF) and XAD-4 resin at Fort McHenry Tunnel (Baltimore, MD, USA) in February and August 2015 to estimate the saturation vapor pressure of about 100 individual semi-volatile organic compounds. The tunnel passes under the Baltimore Harbor and carries traffic for Interstate 95, the main highway on the East Coast of the U.S. The daily traffic volume during this study was approximately 55,000 vehicles per day. Concentrations of individual compounds were determined by extracting TIGF and XAD-4 samples separately and analyzing the extracts using electron impact (EI) GC/MS for polycyclic aromatic hydrocarbons (PAHs), oxy-PAHs, alkanes and cycloalkanes in the range of C12 to C40, and hopanes/steranes. Using gas-particle partitioning theory, we estimated the saturation vapor pressure of individual SVOCs. In general, the estimated values for C12 to C40 n-alkanes agreed well with the available data. We will also present comparison of estimated vapor pressures for other compounds for which literature data is available.

4AC.43

Secondary Organic Aerosol and Organochloride Formation from Alkanes. DONGYU S. WANG, Lea Hildebrandt Ruiz, *University of Texas at Austin*

Alkanes account for nearly 40% of anthropogenic volatile organic compounds emitted each year. Enhanced alkane mixing ratios have been reported within unconventional natural gas production regions. The air quality impacts of anthropogenic alkanes remain highly uncertain due to scarce ambient and laboratory data on the precursor abundance and oxidation product composition, especially for larger alkanes.

Environmental chamber experiments were carried out to investigate the photo-oxidation of linear, branched, and cyclic C_{8-12} alkanes. Nitrogen oxides (NO_x) were added to simulate polluted environments. Chlorine radical was added to simulate early morning oxidation chemistry and effects of atmospheric aging. A High-Resolution Time-of-Flight Chemical Ionization Mass Spectrometer (CIMS) was used to characterize the gas-phase chemical composition. A Filtered Inlet for Gas and AEROsol (FIGAERO) was coupled to the CIMS to collect aerosol and to analyze its molecular composition via thermal desorption. The thermal desorption signal of individual species, when viewed as a function of the desorption temperature, can be used to assess the relative volatility of particulate compounds. As an extension of this 1-D thermogram representation, a 2-D thermogram framework was developed to visualize the particle-phase chemical composition and volatility distribution simultaneously using unit-mass-resolution FIGAERO-CIMS data. A clear correlation between molecular mass and volatility of organic aerosol components was observed using the 2-D thermogram. An Aerosol Chemical Speciation Monitor (ACSM) was used to quantify the SOA mass. The observed SOA yields were much higher than SOA yields previously reported for OH-initiated oxidation of alkanes under high NO_x conditions. A comparison of OH-alkane and chlorine-alkane 2-D thermograms shows that oligomers and highly oxidized organic compounds contributed to the high SOA yield observed for chlorine-initiated oxidation of alkanes. Both FIGAERO-CIMS and ACSM measurements show trace amounts of alkane-derived organochloride reaction products, and a potential formation pathway is proposed. The chamber relative humidity was varied between 0 to 80% to explore its effect on SOA formation. Alkane-derived organochloride formation was suppressed under humid conditions, consistent with the proposed reaction mechanism. Overall, the results suggest that long-chain anthropogenic alkanes could have greater contribution to aerosol loading over its atmospheric lifetime than previously thought.

4AC.44

Gas and Particle Phase Products of the Reaction of 1-Decanol with OH Radicals in the Presence of NOx. ALLISON DAVIS, Xiaoxi Liu, Jose-Luis Jimenez, Paul Ziemann, *University of Colorado-Boulder*

The products and mechanism of secondary organic aerosol (SOA) formation from the OH radical-initiated reaction of 1-decanol in the presence of NOx were investigated in an environmental chamber. Controlled environmental chamber studies provide data concerning gas-phase chemistry as well as gas-particle partitioning and particle-phase reactions, which are necessary for developing detailed chemical models for use in predicting atmospheric fate of volatile organic compounds (VOCs) and SOA formation. Understanding the fate of alcohols in the atmosphere is of increasing importance in rural and urban environments. Alcohols are widely used in industrial solvents and as fuel sources and are emitted into the atmosphere by vegetation. In this study, particle-phase products were analyzed in real time with a thermal desorption particle beam mass spectrometer and off-line following collection onto filters. Subsequent analysis of functional groups by derivatization-spectrophotometric methods developed in our lab allowed quantification of carbonyl, hydroxyl, carboxyl, ester, nitrate, and peroxide functional groups. Derivatized products were also separated by high performance liquid chromatography for molecular quantitation by UV absorbance and identification using chemical ionization-ion mass spectrometry. Identified products consist of highly multi-functional compounds containing various combinations of functional groups and include hydroxydinitrates and dihydroxynitrates, and some also contain an aldehyde group which may promote the formation of low volatility oligomers and cyclic hemiacetals. A suite of experiments employing these methods probed the role of functional groups in aging SOA. Identification and quantification of first, second, and older generation products is necessary for understanding the influence of particle composition on gas-particle partitioning, particle-phase reactions, and SOA properties such as viscosity. Measurements of gas and particle phase products of alcohol oxidation also offer insight into the chemical mechanism and physical processes leading to SOA formation.

4AC.45

Secondary Organic Aerosol Formation of OH and NO3 Initiated Reactions of 1,3-Benzenediol. ZACHARY FINEWAX, Joost de Gouw, Paul Ziemann, *University of Colorado*

Biomass burning is the second largest emission source of volatile organic compounds (VOCs) and largest of particulate matter (PM) globally. Previous studies measuring emissions from biomass burning have identified 1,3-benzenediol (resorcinol), a semi-volatile organic compound (SVOC) emitted as a pyrolysis product of lignin, a biopolymer found in wood. To date, there have been no studies on the gas-phase oxidation of this compound, which may be an important precursor for secondary organic aerosol (SOA) from biomass burning.

To study the reactions of resorcinol that could occur in a biomass burning plume, OH and NO_3 radical-initiated reactions (simulating daytime and nighttime, respectively) of resorcinol in the presence of NO_x were conducted in an 8 m^3 FEP Teflon environmental chamber operated in batch mode. OH radical-initiated reactions were performed by photolysis of methyl nitrite (CH_3ONO) in the presence of NO by blacklights, and NO_3 radical-initiated reactions were performed by thermal decomposition of N_2O_5. Because of the low volatility of resorcinol and thus potential for loss to the chamber walls, studies of the gas-phase chemistry were conducted by adding resorcinol while photolysis of CH_3ONO or thermal decomposition of N_2O_5 was already occurring in the chamber. This allowed for reaction to occur prior to wall loss because of the high reactivity of resorcinol with both oxidants. SOA produced by these reactions was measured with a thermal desorption particle beam mass spectrometer (TDPBMS) and scanning mobility particle sizer (SMPS), and was collected on Teflon filters to quantify the SOA yield. The gas-phase compounds were measured and quantified by Proton-Transfer-Reaction Mass Spectrometry (PTR-MS) and collection onto denuders to quantify VOCs, and SVOCs that exist in both the particle and gas-phase. Molecular identification and quantification was conducted by high-performance liquid chromatography (HPLC) and chemical ionization ion trap mass spectrometry (CI-ITMS) on SOA filter and denuder extracts through the use of commercially available and authentic standards collected from HPLC fractions.

SOA and molecular yield calculations assumed complete reaction of the added resorcinol, which is appropriate given the calculated kinetics of resorcinol reactions with OH and NO_3 radicals, and the expected much longer timescale for vapor wall loss in the environmental chamber. The product distribution of the SOA from OH-initiated reactions is dominated by 1,2,3-benzenetriol and 1,2,4-benzenetriol, with minor contributions from benzenetetraols, 5-nitro-1,2,3-benzenetriol, and nitroresorcinol isomers. In the OH radical reaction, hydroxybenzoquinone and dihydroxybenzoquinone are generated as gas-phase products both by gas-phase reaction and multiphase chemistry involving oxidation of benzenetriols and benzenetetraols by nitric acid. This was determined through additions of ammonia, and monitoring the reduced loss of benzenetriols from the particle phase. The SOA mass yield of 0.61 for the OH radical-initiated reaction was over a factor of 2 higher than the yield of 0.27 from the NO_3 radical-initiated reactions, while the products were 4-nitroresorcinol, 2-nitroresorcinol, and hydroxybenzoquinone. The presence of nitroresorcinol in both the gas-phase and particle-phase indicate that these compounds are semivolatile. The results of this study highlight the importance of resorcinol oxidation to SOA formation during the day compared to at night.

4AC.46

Clustering Process of Glyoxylic Acid Involving Gas-phase Hydration Reaction: Implications for the Atmospheric Models. Ling Liu, Oona Kupiainen-Määttä, XIUHUI ZHANG, *Beijing Institute of Technoloy*

Atmospheric aerosol nucleation mechanism is important but still not clear, especially different reactivities of precursors can induce various chemical reactions during the clustering process besides the cluster formation through hydrogen bond. However, chemical reactions are not fully considered in most of the nucleation processes. Herein, the clustering process of glyoxylic acid (GA), the most abundant oxocarboxylic acids in the atmosphere, involving gas-phase hydration reaction are studied by Density Functional Theory combined with Atmospheric Clusters Dynamic Code. The hydration reaction of GA can occur in clustering process with the conversion ratio up to 85%, and the product can further participate in the clustering process. GA with its hydration reaction can enhance cluster formation rate. The differences in cluster structure and property induced by hydration reaction lead to the discrepancies in cluster formation rates and pathways. These results shed some light on the discrepancy between atmospheric models and field measurements and have important implications for atmospheric model improvement.

4AE.1

Reactive Oxygen Species (ROS) Activity Map Induced by PM2.5 in 10 Different Cities, China. SHEXIA MA, Yanshan Lv, Xiaoying Li, Yangyang Zhang, Xuejun Liu, Mei Zheng, *South China Institute of Environmental Sciences, MEP*

Numerous epidemiological studies have confirmed that exposure to ambient fine particulate matter (PM2.5) may increase cardiopulmonary mortality and morbidity. Oxidative potential (the ability of ambient particles to generate ROS) is a more relevant measurement when attempting to link aerosols and health end points. In this study, we quantify the oxidative potential of ambient particles collected during four seasons in 10 cities, China, using the dithiothreitol (DTT) assay, and aim to investigate the spatial and seasonal heterogeneity of ROS induced by PM2.5 in China. We find that PM2.5 are generally more reactive in clean days (<75µg/m3) than in polluted days (>75µg/m3), the increased health risk is gradually reduced per unit PM2.5 mass when PM2.5 concentration was above 75µg/m3. Annual average of blank-corrected DTT loss ranged from 1.42 to 25.50 pmol DTT min-1µg-1 PM among the 10 sites with a mean of 6.122±7.086 pmol DTT min-1µg-1 PM. The highest DTT activity was observed at the Guangzhou and the lowest occurred at the Baoding, with the ratio of average DTT loss is 5.25. The spatial distribution of DTT activity generated by PM2.5 collected in 10 different cities shows that higher DTT loss in coastal sites such as Guangzhou, Dalian, Fuzhou etc., lower DTT loss in inland sites, such as Baoding, Dezhou, Handan etc, which is the first spatial ROS activity map in China. There is a clear seasonal variation with highest activity in summer and lowest activity in spring, the average ratio of 1.97, indicated different sources and chemical properties of PM2.5 had significant effect on ROS generation. Slightly higher relative risks (RRs) of ambient PM2.5 were observed in Guangzhou and Dalian with lower PM2.5 level, while the lowest RRs were observed in Beijing with higher PM2.5, which was consistent with ROS activity map in the present study, suggesting that smaller particles, which might contain more toxins from anthropogenic emissions, can more easily reach the acinar part and promote oxidative stress and inflammation.

4AE.2

Indoor-Outdoor Particulate Relationship and Its Metal Bound Concentrations in Domestic Homes of 'World Heritage Site' Agra, India. HIMANSHI ROHRA, Ajay Taneja, *DR. B.R.A. University, Agra, India*

The present work endeavours to parade the influence of particle size and associated metals (Al, Ba, Ca, Cu, Fe, K, Mg, Mn, b, Cd, Co, Zn) within coarse (2.5-10µm), accumulation (2.5-0.25µm) and ultrafine (UF) (<0.25µm) particulate matter (PM) ranges in living rooms of residential homes with their subsequent comparison with outdoor levels at Agra, India. Higher PM concentrations were measured through cascade impactor in indoors (PM10= 264 µg/m3; PM2.5= 195 µg/m3) as compared to outdoors (PM10= 212 µg/m3; PM2.5= 153 µg/m3); both surpassing the WHO benchmark targets. In view of size segregated aerosol, q-UF particles dominated indoor (37%) and outdoor (28%) concentration levels; accounting as major health concern. Poor relationship between indoor-outdoor particle sized levels and coarse and fine PM indicate heterogeneity of sources in concurrent with wash out of particles during precipitation events in sampling tenure. A unimodal lognormal distribution of PM was obtained with preference to droplet mode peak (1.0-0.5µm) in outdoors that shifted to smaller size (0.5-0.25µm) in indoors. For K, Co, Zn, modal shifting in indoor vs outdoor aerosol distribution were observed. The applied regression model further inspected the infiltration capacity of varied particle size modes in different housing conditions. Shifting of particles towards q-UF range in indoors of roadside homes impacted resident exposure to toxic particles. This work prerequisites in designing pollution control strategies to achieve a healthier indoor living environment in this area.

4AE.3

Effect of Particle Morphology on Performance of an Electrostatic Air–Liquid Interface Cell Exposure System. TA-CHIH HSIAO, Jing-Chi Lin, Hsiao-Chi Chuang, Tsun-Jen Cheng, *National Central University*

The particle morphology can affect the performance of electrostatic-precipitator air–liquid interface (ESP-ALI) cell exposure system as well as cell toxicity. In this study, three types of monodisperse aerosols—spherical sucrose particles, nonspherical soot aggregates, and silver aggregates/agglomerates—were selected to evaluate the collection efficiency at a flow rate ranging from 0.3 to 1.5 lpm. To quantify the particle morphology, the fractal dimension (Df) of testing aerosols were characterized. At identical conditions, the penetration rate for fine particles (dp = 100–250 nm) under different operating conditions was correlated with a characteristic exponential curve using a dimensionless drift velocity (Vc/Vavg,r) as the scaling parameter. For ultrafine particles (UFPs, dp< 100 nm) with different particle morphologies, the particle penetrations in the ESP-ALI were similar, but their diffusion losses were not negligible. By contrast, for fine particles, the collection efficiency of soot nanoaggregates (Df = 2.29) was higher than that of spherical sucrose particles. This might be due to the simultaneous influences of the electric field–induced alignment and the flow field–induced alignment. Furthermore, based on Zhibin and Guoquan's Deutsch model, a quadratic equation was applied to fit the experimental data and to predict the performance of the ESP-ALI.

4AE.4

Determination of Inhalation Exposure due to the Use of Eyebrow Powders. HYEON-JU OH, Taewon T. Han, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

Consumers may be exposed to inhalable aerosols when they apply cosmetic products; however little is known about the extent of such exposures. Here we investigated inhalation exposures when applying five types of eyebrow powders using two types of brushes and determined the mass-based inhaled and deposited aerosol dose. For this project, the powers were applied to mannequin's eyebrows in a realistic manner. The "inhaled" aerosol was sampled through two stainless-steel tubes installed in the mannequin's nostrils for real-time measurement by a Grimm optical particles counter (model 1.108, Grimm Technologies Inc., Douglasville, GA) and collected on filters for gravimetric analysis. The aspiration rate through the nostrils of the mannequin was 10.8 L/min. Experiments with each product were repeated three times. The Grimm measured the inhaled particulate matter (PM) mass concentration for Total Suspended Particles (TSP), PM10, and PM4, and particle size distribution; a cyclone (GK 2.69, Mesa Labs, Inc.) was used to collect PM10, and PM4 inhaled powder fractions. The original powders and the fractions of airborne powders (PM10 and PM4) were characterized using a scanning electron microscope (SEM) (FESEM, Zeiss Sigma). The concentrations measured by the Grimm were 120.5 – 334.4 µg/m3 (TSP), 56.04 – 206.4 µg/m3 (PM10), and 22.2 – 46.8 µg/m3 (PM4), while the concentrations measured by gravimetric analysis were 134.6 – 277.3 µg/m3 (TSP), 43.7 – 136.9 µg/m3, (PM10) and 21.2 – 53.7 µg/m3 (PM4). When deposition by mass was calculated using ICRP deposition model, most of the inhaled powder mass deposited in the head airways (almost 79%), while less than 6% of deposition occurred in the alveolar region. The SEM analysis showed the presence of nanoparticles and their agglomerates in the original and airborne state of all powder products. The results show that determination of potential exposure to respirable particles stemming from cosmetic powder application is feasible through a realistic simulation. In addition, the data show that the concentrations of particulate matter fractions inhaled during eye powder applications could be quite substantial. Future studies will consider potential health effect due to such short-term exposures.

4AE.5

Personal Exposure Monitoring Using Integrated Sensors and Cloud Computing. SEPEHR MAKHSOUS, Angela Chavez, Igor Novosselov, Alexander Mamishev, *University of Washington*

Direct measurements of time and size-resolved particle concentrations are of major importance personal exposure assessments, air quality studies, and pollution monitoring. Human exposure to particulate matter (PM) is associated with multiple adverse health effects including cardiovascular disease, cardiopulmonary disease, and lung cancer. A variety of methods is currently used to measure particle concentrations, including traditional gravimetric filters, aerodynamic particle sizers, beta attenuation monitors and scanning electrical mobility sizers. These methods are highly accurate, but their large size and high price make them impractical for use as personal monitors or area monitor that can be used for detailed mapping of the occupational exposure. Applications demand more practical instruments that are compact, automatic, and low-cost without forgoing sizing accuracy and reliability. Additionally, information about real-time spatial and temporal distribution PM concentrations is essential to prevent exposure and create more effective intervention strategies. Integrated Sensors and Cloud Computing (ISCC) platform provides personal PM exposure assessment. We present the development and evaluation of a low-cost PM ISCC system which uses compact, low-cost Optical Particle Counter (OPC) integrated with an ATMEL microcontroller, a Bluetooth module, and a Wi-Fi chip installed on a Printed Circuit Board (PCB.) The monitor is connected to a smartphone mobile application that allows the user to access data in real time or store it for future examinations. Results of the test show that the system is capable of identifying and classifying PM in real time. Multiple monitors can be connected to a secured cloud for real-time mapping of the facility allowing to take preemptive actions and avoid hazardous health episodes.

4AE.6

Exposure to Polycyclic Aromatic Hydrocarbons (PAHs) in PM10 at Urban Area of a Semi-Arid Region of India. AMIT MASIH, *St. Andrew's College, Gorakhpur, India*

Polycyclic Aromatic Hydrocarbons (PAHs) are toxic air pollutants (TAPs) that have the potential to cause serious and adverse health effects and damage to the environment. These pollutants differ from other primary air pollutants such as sulphur dioxide, nitrogen dioxide, total suspended particulates (TSP) and respiratory suspended particulate matter (RSPM) in the respect that even at substantially lower concentrations; their health effects are carcinogenic in nature. Particulate matter from an urban residential site within Agra city (a semi-arid region) were collected using respirable dust samplers for a span of one year (2010-2011) in order to study the concentration and exposure profiles of PAHs. The samples were extracted with dichloromethane using an automated Soxhlet Extraction. The extracts were analyzed for 17 target Polycyclic Aromatic Hydrocarbons (PAHs). The total PAH (TPAH) concentrations were 27.96 ± 2.3, 22.24 ± 2.1, and 34.38 ± 3.0 ng m-3, respectively, during summer, monsoon and winter seasons. The combined mean concentration of TPAH was 28.19 ngm-3 for all seasons. Benzo(b)fluoranthene, Benzo(g,h,i)perylene, Benzo(b)fluoranthene and Indeno(1,2,3-cd)pyrene were the chief PAHs found in the samples collected from this urban region. The average TPAH percentage based on the number of rings were 1% (2-ring), 2% (3-ring), 24% (4-ring), 48% (5- ring), and 25% (6-ring). Dibenz(a,h)anthracene contributed the highest carcinogenic exposure equivalent (4.09 ng m-3) followed by Benzo(a)pyrene (2.80 ng m-3), Benzo(b)fluoranthene (0.453 ng m-3) and Benzo(k)fluoranthene (0.338 ng m-3), accounting for approximately 50%, 35%, 6% and 4% of the total carcinogenicity of particulate PAH in this urban region, respectively.

Keywords: Particulate Matter, PAH, Carcinogenic Potencies, Semi Arid Region

4AE.7

Data Requirements for Mapping Long-Term Air Pollution with Mobile Short-Term Measurements. RIVKAH GARDNER-FROLICK, Joshua Apte, Kyle Messier, *University of Texas at Austin*

New large-scale approaches to air quality data collection have the potential to substantially advance understanding of human exposure to outdoor air pollution, which varies sharply in space and time. For example, some methods use mobile monitors or temporarily stationed sensors to provide highly spatially resolved data. One inherent limitation is that these methods provide sparse temporal resolution for any given location, raising the question of their ability to monitor long-term trends. Here, we investigate whether a series of short-term measurements can adequately represent long-term average concentrations at a monitoring site. To do so, we conduct a Monte Carlo subsampling analysis of 2011-2017 Bay Area Air Quality Management District (BAAQMD) 1-hour measurements of black carbon (BC), nitric oxide (NO), nitrogen dioxide (NO_2), fine particulate matter ($PM_{2.5}$), carbon monoxide (CO), sulfur dioxide (SO_2), and ultrafine particulate matter (UFP) at multiple locations in the San Francisco Bay Area, California and 2012-2014 Southeastern Aerosol Research and Characterization (SEARCH) Network 1-minute measurements of BC, NO, NO_2, and CO in Atlanta, Georgia. Methods developed using the BAAQMD and SEARCH data ultimately will be applied to air pollution data collected in the San Francisco Bay Area using Google Street View cars. In this dataset, 1-Hz measurements of air pollution are matched to the nearest 30-meter road point and analyses can be performed for each location or for larger road segments.

We use random and structured subsampling to estimate the number of observations needed to achieve an accurate (within ±10%) estimation of the annual mean. The geometric standard deviation of continuous measurements, for both 1-minute and 1-hour time intervals, is descriptive of air quality at a site and is highly predictive of the number of samples required to estimate the mean for a specific pollutant at that site. Across all locations, pollutants tend to cluster together, having a similar geometric standard deviation and required number of samples. The pollutant with the lowest number of required samples is CO, which requires 32 independent observations. The pollutant with the highest required number is NO, with 428 samples. While pollutants tend to cluster together across all monitored locations, a few points have significantly different required sample numbers. For example, the average required sample number for BC is 112, while the required sample number at the Forest Knolls site is 490. These breaks in clustering can be attributed to extremely variable seasonal and diurnal patterns, with the breaks occurring at a given location in a predictable manner. These overall trends hold for both random and structured sampling schemes, corresponding to different real-world field study designs. Given the highly correlated nature of air quality measurements, we found that independent measurements are more important than the length of the measurement period. The results hold important implications for future air quality study design and the practicality of using disparate monitoring methods to collect the most useful information. A small number of discrete measurements, such as those gathered from mobile monitoring, can be highly predictive of annual averages.

4AE.8

Impacts of E-Cigarettes Consumptions on the Air Quality of Vape Shop and Its Nearby Areas. LIQIAO (VICKY) LI, Charlene Nguyen, Yan Lin, Yifang Zhu, *University of California, Los Angeles*

With the rapid growth of e-cigarette (e-cig) market in the U.S, there is an increasing number of independent retail specialty shops (vape shops) that exclusively sell e-cig. The consumption of e-cig in the vape shop might bring a new emission source for aerosol exposure in its indoor environment and nearby businesses. In this study, we selected a representative vape shop in Los Angeles and recorded the number of vaping puffs in every 10 minutes in the shop for four days. Meanwhile, we measured real-time $PM_{2.5}$ concentration and particle number concentration (PNC) in the vape shop as well as its nearby business (~ 3 m away) and outdoor area (~6 m away). Weekly average nicotine concentrations were also measured in each site. The average concentration (SD) of $PM_{2.5}$, PNC and nicotine in the vape shop was 426 (1283) microgram/m^3, 1.89 (2.14)*10^4 /cm^3, and 1.71 microgram/m^3, respectively, which were much higher than those in nearby business (i.e. $PM_{2.5}$: 16.3 (9.3) microgram/m^3; PNC: 8.42 (19.7)*10^3 /cm^3; nicotine: 1.29 microgram/m^3) and outdoor areas (i.e. $PM_{2.5}$: 17.2 (14.0) microgram/m^3; PNC: 8.96 (5.04)*10^3 /cm^3). The number of vaping puffs were significantly correlated with $PM_{2.5}$ concentration ($r=0.74$, $p<0.001$) and PNC ($r=0.71$, $p<0.001$) in the vape shop, indicating the significant contribution of e-cig consumption to indoor aerosols. On the day with the highest average puff number, $PM_{2.5}$ and PNC in the vape shop were significantly correlated with those in nearby business and outdoor area ($p<0.05$), suggesting the impacts of vape shop on nearby air quality. Thus, the secondhand emissions of aerosols in the vape shop potentially impacted on both its and nearby indoor environment.

4AE.9

Personal Exposure to Particulate Matter While Commuting. VÂNIA MARTINS, Susana Marta Almeida, Tiago Faria, Carolina Correia, Inês Cunha-Lopes, Nuno Canha, Evangelia Diapouli, Manos Manousakas, Konstantinos Eleftheriadis, *C2TN, IST, Universidade de Lisboa, Portugal*

Numerous epidemiological studies have demonstrated associations between traffic-related air pollution exposure and a variety of negative human health outcomes. As more commuters are spending a considerable amount of their daily routine inside vehicles it is increasingly relevant to study exposure levels to harmful pollutants. Depending on pollutant, mode of travel and travel distance, the exposure while commuting during along trafficked corridors may constitute a substantial fraction of the total daily exposure. Information regarding the air quality variations when commuting through a city can help the citizens to make more informed decisions on possible avoided emissions when choosing a transport mode and reduce their exposure to air pollutants.

This study aims to assess urban air quality experienced during commutes on different transportation modes. Continuous measuring portable monitors were used during journeys through the city of Lisbon by bus and car. The study continuously tracked not only particles mass and number and black carbon during each journey, but also included collection of PM2.5 and PM10 samples using Personal Environmental Monitors. The chemical characterisation of the PM collected on the filters was carried out in order to assess the commuters’ exposure to PM components.

The values found inside the vehicles when commuting were higher than those measured at urban background monitoring stations, a fact which underlines the need to assess personal exposure by acquiring data directly in the microenvironments where people spend their time.

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4AE.13

Uptake of Tobacco Related Reduced Nitrogen Species to Aqueous Aerosols. PETER DECARLO, Anita Avery, Erin Katz, Michael Waring, *Drexel University*

Indoor and outdoor summertime measurements of aerosol composition identified a unique organic signature in the indoor dataset. Measurements of organic aerosol composition in an unoccupied classroom showed a high fraction of the organic mass was attributed to reduced nitrogen species identified by ions in the mass spectra of the general formula: $C_xH_yN_z$. Positive Matrix Factorization of the organic aerosol showed 25-29% of the indoor aerosol was attributable to this indoor source. Through subsequent controlled laboratory experiments, these reduced nitrogen related ions were identified as originating from aged residual tobacco smoke volatilizing from surfaces or clothing in the indoor environment. Controlled laboratory experiments using deposited tobacco smoke in a pyrex vessel in coordination with observational data provided evidence of reactive uptake through acid base chemistry. Further experiments with deposited e-cigarette emissions showed similar behavior initially, but with increasing residence time, e-cigarette residue resulted in stable chemical signatures of nicotine and other e-cigarette liquid constituents (glycol and flavorings) compared to the chemical transformation observed for cigarette residue. While the results are generated from indoor observation of these species, the acid-base reactive uptake mechanism of reduced nitrogen species is applicable to outdoor aerosols and expected to be important in areas where amines and other reduced nitrogen compounds are prevalent.

4AE.14

Community-Level Spatial Mapping of Ultrafine Particle Number Concentration. PRADEEP S. PRATHIBHA, Ray Yeager, Aruni Bhatnagar, Jason S. Su, Jay R. Turner, *Washington University in St. Louis*

The Green Heart Project is a prospective study examining linkages between urban vegetation and cardiovascular health. This association could be mediated by several factors, including the effect of vegetation on local air quality. The study is being conducted in Louisville, KY, where a 1900-acre region has been chosen for long-term monitoring of major urban air pollutants. A 575-acre contiguous region within the domain serves as the intervention area where mature vegetation selected based on ecological compatibility and pollutant abatement characteristics will be installed for near-road as well as widespread neighborhood-scale ‘greening’. The remainder of the study domain serves as the non-intervention (control) area. As part of this study, we are estimating residential level exposure to ambient air pollution with measurements being conducted in the intervention and control areas both before (baseline) and after planting.

To date, pilot studies have been conducted in the control and intervention areas using a mobile platform with ultrafine particle (UFP) number concentration measured at one-second time resolution. An interstate highway with ~4 m high noise barrier bisects the study domain, and rush hour UFP concentrations <10 m downwind of the barrier were up to 45 times greater than background levels. Consistent with previous studies, UFP concentrations returned to background levels within a short distance (<150 m) of the highway. Measurements are also conducted along major arterial roadways and residential streets, and repeated under varying traffic and dispersion conditions. In spring 2018, baseline measurements will expand to include black carbon (BC) and CO_2 on the mobile platform and NO_x ($NO + NO_2$) through a time-integrated passive sampler network; additional parameters will be added as the study progresses. A vegetation planting strategy informed by the baseline measurements will be implemented in fall 2018; post-intervention air quality measurements will be conducted thereafter.

4AE.15

Exposure of Children to Particulate Matter and Chemical Elements in Urban Environment. Tiago Faria, Marina Almeida-Silva, VÂNIA MARTINS, Inês Cunha-Lopes, Carolina Correia, Catarina Galinha, Célia Alves, Susana Marta Almeida, *C2TN, IST, Universidade de Lisboa, Portugal*

Introduction

Particulate matter (PM) is a concern due to the adverse health effects it causes on human health. These effects are linked to the chemical components particles contain and their size and the efficiency of pulmonary deposition. Children spend more than 80% of their time indoors. Therefore, it is necessary to develop the best strategies to reduce PM exposure in various microenvironments in order to reduce health effects. The objective of this study was to quantify the daily exposure of children to PM and their chemical compounds considering different size fractions.

Methodology

Ten children aged 5 to 9 living and studying in the city of Lisbon were selected to be part of this study using personal particle samplers for 3 days.

The particles were collected on Teflon filters using a personal cascade impactor (PCIS) connected to a Leland Legacy SKC pump which sampled particles in the size ranges <0.25, 0.25-0.5, 0.5-1, 1-2.5 and > 2.5 µm. The mass concentrations of the particles were determined gravimetrically. All samples were chemically analyzed by ICP-MS in order to determine the concentration of major and trace elements present in PM. In addition to this sampler, the children carried a monitor to make real-time measurements of PM2.5 concentrations, a particle number counter to measure the number concentration of particles between 10nm and 1µm, and a microaethalometer to measure black carbon concentrations. These equipments were accompanied by a GPS that registered the coordinates of the routes of the children. At the same time, the children fill a logbook every 15 minutes, indicating the main activities carried out indoors and outdoors, as well as the activities carried out by others that can affect the exposure, such as food confection or smoking.

Results

The results of activity logs and GPS were combined with the mass and numerical concentrations of PM and black carbon in order to identify the microenvironments that contributed most to children's exposure. The analysis of the filters allowed to evaluate the size distribution of the particles and to calculate the children's exposure to different chemical elements. The inhaled dose was calculated considering the measured concentrations, the time activity patterns of each child and the inhalation rate. The results showed the importance of the indoor environment, especially of the house and the classroom, for children's exposure to particles.

Conclusions

This study allowed understanding the children exposure to PM in the various microenvironments where they remain and the respective inhaled dose. The study of the particle size distribution and their chemical constituents was an essential input for dosimetry models that aim to evaluate the particles that reach the different regions of the body and thus estimate potential health effects.

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4AE.16

Characterization of Nanoparticle Containing Formulations before and after Spraying on Textile Surfaces: The Influence of Surface Active Substances on Aerosol Formation Relevant for Inhalation. FRANK BIERKANDT, Sandra Wagener, Jutta Tentschert, Harald Jungnickel, Peter Laux, Andreas Luch, Lars Hillemann, Paul Bergelt, *Federal Institute for Risk Assessment (BfR)*

The growing application of engineered nanomaterials (ENM) and especially the use as constituents in numerous spray products (e.g., cosmetics, coating or cleaning products) increase the possibility of human exposure via inhalation. A detailed investigation of their behavior and toxic potential is therefore necessary. Adverse effects associated with aerosol inhalation are connected to the size and shape of ENM (e.g., rod-like particles) - amongst others - as these factors influence accessibility within the lungs. Moreover, the composition of the sprayed formulation and the resulting aerosol can also impact the toxicity as compounds adsorbed on any ENM may alter its properties as e.g. cellular uptake or reactivity. Also, certain formulations may carry substances into areas which are normally inaccessible (i.e., Trojan Horse effect). Thus, characterization of spray formulations and their influence on the fate of ENMs in solution as well as after aerosolization is essential and shall be addressed in this work. In addition to this, the alteration of the ENMs upon uptake in cellular systems will be investigated, combined with toxicity testing.

The emulated spray formulations - based on pure water and ethanol - contain Ag- and CeO_2-ENMs in combination with several additives. These particles were selected because of their frequent use based on their bactericide activity (Ag-ENMs) or their UV-stability (CeO_2-ENM). They also represent two groups of ENMs with different solubility: while Ag-ENMs are more soluble, CeO_2-ENMs are considered rather insoluble and biodurable. To address nanoscale effects, respirable ENM sizes of < 100 nm, ~ 200 nm in addition to microsized particles were tested. Because surface active substances are sometimes used to alter the spray behavior, the influence of two perfluorinated silanoles on the ENM toxicity is being tested exemplarily.

The mentioned formulations were analyzed in regard to any alterations on the ENM characteristics before aerosolization and also after spraying onto textiles in order to simulate an impregnation process. Single particle inductively-coupled plasma mass spectrometry (spICPMS) and dynamic light scattering (DLS) were used for analysis in solution. For analysis of sprayed samples, time-of-flight secondary ion mass spectrometry (ToF-SIMS) as well as laser ablation (LA)-ICP-MS were applied.

First results indicate alterations induced in the ENM characteristics regarding size distribution and their dispersion stability by the different formulations. Time-resolved sp-ICP-MS analysis shows decreasing NP sizes for some ENM-formulations.

Using LA-ICP-MS of sprayed textiles, a distinction between different pre-treatments of textile samples could be seen in regard to ENM agglomeration after aerosol application onto these textiles. Using ToF-SIMS analysis penetration depth of applied ENMs to about 1 µm into the textile could be proofed and an aggregation size between 100 nm and 1 µm was recorded whereas the ENMs emitted from the source were sized below 100 nm.

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4AM.1

The Basics of Taylor Series Expansion Method of Moment for Brownian Coagulation. MINGLIANG XIE, *Huazhong University of Science and Technology*

In this paper, we will introduce the new development of Taylor series expansion method of moment (TEMOM) for Brownian coagulation, such as the error estimation of TEMOM, the asymptotic solution of TEMOM, and the physical constraint of Brownian coagulation, etc.

These results will help us in understanding the Brownian coagulation and population balance equation.

4AM.2

Effects of Airway Surface Roughness on Local Particle Deposition in Subject-Specific Tracheobronchial Trees. YU FENG, Xiaole Chen, Jianan Zhao, Arvind Santhanakrishnan, *Oklahoma State University*

Computational Fluid-Particle Dynamics (CFPD) models are useful are useful and efficient to understand inhaled aerosol dynamics in human respiratory systems. Crucial to such models is the accuracy of predicting particle depositions. Reconstructed from CT/MRI scanned data, subject-specific human airway configurations are widely used in computational lung aerosol dynamics research. Smoothing the airway surfaces is inevitable during this process. However, the smoothing criteria used are inconsistent among research groups, which may lead to errors in particle deposition results. To investigate the roughness effect and enhance the reliability of the CFPD model, this research simulated the transport and deposition of inhaled particles in 3 tracheobronchial trees reconstructed from the same CT data for a healthy subject with different smoothing intensities. The inhalation flow rate ranges from 30 L/min to 120 L/min, and the particle size is from 50 nm to 10 µm. Numerical results indicate that improper smoothing process will underpredict particle deposition fractions up to 50% in the trachea, which is due to the underestimated turbulence fluctuation effect on particle deposition. In contrast, it is interesting to notice that the roughness effect on particle depositions from Generation 2 (G2) to Generation 6 (G6) is negligible. In conclusion, smoothing process has a significant impact on laminar-to-turbulence transition and local turbulence intensity, thereby influencing particle deposition result variations in the trachea. To employ a proper smoothing process to reconstruct the 3D lung airway geometries for *in silico* studies, it is necessary to accurately measure the airway surface roughness considering the presence of mucus layers. To build a more accurate and realistic *in silico* model for lung aerosol dynamics research, a generalized and unified guideline of the smoothing procedure will be developed based on the extensive intersubject variability studies among virtual population groups with statistical robustness.

4AM.3

Development and Experimental Validation of Coupled Flow-Aerosol Dynamics Model for a Glowing Wire. KUNAL GHOSH, S.N. Tripathi, Manish Joshi, Y.S. Mayya, Arshad Khan, B.K. Sapra, *IIT Kanpur*

We have developed a CFD coupled aerosol microphysics model in context of aerosol generation from a glowing wire. The governing equations can be solved implicitly for mass, momentum, energy transfer along with aerosol dynamics. The computationally efficient framework can simulate temporal behavior of total number concentration and number size distribution. This formulation uniquely couples standard K-Epsilon scheme with boundary layer model with detailed aerosol dynamics through residence time. This model uses measured temperatures (wire surface and axial/radial surroundings) and wire compositional data apart from other usual inputs for simulations. The model predictions show that bulk fluid motion and local heat distribution can significantly affect the aerosol behavior when buoyancy effect in momentum transfer is considered. Buoyancy generated turbulence was found to be affecting parameters related to aerosol dynamics and transport as well.

The model was validated by comparing simulated predictions with results obtained from six controlled experiments performed with a laboratory made hot wire nanoparticle generator. Condensation particle counter (CPC) and scanning mobility particle sizer (SMPS) were used for measurement of total number concentration and number size distribution at the outlet of reactor cell during these experiments. Our model-predicted results were found to be in reasonable agreement with observed values.

The developed model is fast (fully implicit) and numerically stable. It can be used specifically for applications in context of behavior of aerosol particles generated from glowing wire technique and in general for other similar large scale domains. Incorporation of CFD in aerosol microphysics framework provides a realistic platform to study natural convection driven systems/ applications. Aerosol dynamics sub-modules (nucleation, coagulation, wall deposition) have been coupled with Navier Stokes equations modified to include buoyancy coupled K-Epsilon turbulence model. Coupled flow-aerosol dynamics equation was solved numerically and in implicit scheme. Wire composition and temperature (wire surface and cell domain) were obtained/measured, to be used as input for the model simulations. Model simulations showed significant effect of fluid properties on the dynamics of aerosol particles. The role of buoyancy was highlighted by observation and interpretation of nucleation zones in the planes above the wire axis. The model was validated against measured temporal evolution, total number concentration and size distribution at the outlet of hot wire generator cell. Experimentally averaged and simulated total number concentrations were found to match closely, barring values at initial times. Steady state number size distribution matched very well for sub 10 nm particle diameters while reasonable differences were noticed for higher size ranges. Although tuned specifically for the present context (i.e. aerosol generation from hot wire generator), the model can also be used for diverse applications e.g. emission of particles from hot zones (chimneys, exhaust), fires and atmospheric cloud dynamics.

4AM.4

Calculating Wet Deposition and Aerosol Sizes Sensitivities within a Lagrangian Particle Dispersion Code. LI KAIBO, Xu Xuefeng, *China Academy Of Engineering Physics*

This paper describes an investigation into the uses of first-order, local sensitivity analysis in a Lagrangian dispersion code. The goal of the project is to gain knowledge not only about the sensitivity of the dispersion code predictions to the specific input parameters of interest, but also to better understand the uses and limitations of sensitivity analysis within such a context. The dispersion code of interest here is RATRANS, which is used for modeling emergency release scenarios in nuclear accident. Monte Carlo and ensemble techniques are available in RATRANS. Sensitivity analysis is being explored as a means to gain an understanding of the contribution to uncertainty from certain types of input parameters. As a first step, first-order sensitivity analysis was implemented within the precipitation-scavenging module of RATRANS. This module is logically split from the remainder of the dispersion calculation, so the sensitivities may be explored without concern about parameter and computational dependencies, and the linearization implicit in the formulation is acceptable. The general goals of the project are: To understand the sensitivity of RATRANS predictions of precipitation scavenging (wet deposition) to the rain rate and aerosol particle size; To explore the advantages and limitations of first-order sensitivity analysis within a Lagrangian dispersion framework; To gain the understanding necessary to plan a more comprehensive uncertainty analysis project for the RATRANS suite of codes.

4AM.5

Effects of North California Wildfire in October 2017 on Air Quality and Human Health. FENGLIN HAN, Hongliang Zhang, *Louisiana State University*

The October 2017 Norther California Wildfires were a series of over 250 wildfires across the state of California, resulting in severe environmental and economic loss. This study aims to determine transport of and effects of wildfire emissions based on observed data and chemical transport model. The observational data of meteorology and air pollutants including fine particulate matter (PM2.5) are obtained from California Air Resources Board (ARB) sources. Six stations under direct impact with available PM2.5 data were selected. The Community Multiscale Air Quality (CMAQ) model (v5.2) is also applied with anthropogenic emissions from the National Emissions Inventory (NEI) 2014 using the Sparse Matrix Operator Kernel Emission (SMOKE) model (version 4.5). The fire inventory from National Center for Atmospheric Research (NCAR) is used for emissions of wildfires. Spatial and temporal variations wildfire related air pollutants will also be analyzed and contributions of the wildfires will be quantified. The health and economic effects of the wildfires will also be estimated. This study can provide important information for wildfire-related air quality issues and future health studies.

4AM.6

Coarse, Fine and Ultrafine Particles of Sub-urban Continental Aerosols. DRAGANA ĐORđEVIć, Jelena Đuričić-Milanković, Ana Pantelić, Srđan Petrović, Andrea Gambaro, *CEEC – ICTM, University of Belgrade*

The first investigation of size-segregated sub-urban aerosols from the continental part of the Balkan peninsula in 11 fractions in the range of $0.0085 < D_p < 16$ µm was performed from March 2012 to December 2013. Aerosols were measured at the Zeleno Brdo observatory (44° 78' 61" N, 20° 52' 22" E – 243 m above sea level), which is the highest point near Belgrade on its eastern edge, surrounded by wooded vegetation, with rural areas on its southern parts and urban areas on its north-western part. About 70% of total aerosols are fine particles, belonging especially to the PM0.53–1.06 fraction which is more intensive in the winter period. In this work, we applied tests of probability function models, for three distributions: normal, log-normal and three-parameter Weibull, by comparing expected and observed values. This model offered us the possibility to assess whether it is the dominant emission source in the vicinity of the measuring point or it is distant. Results of this test could be a significant supplement to existing multivariate mathematical models for source apportionment for more accurate estimation of the origin of emission sources, offering information on their position relative to the investigated area (local, regional or remote). The dependence of particle concentrations for each fraction investigated versus meteorological parameters was determined.

4AM.7

Consideration of Wildfires as a Source of Airborne Mineral Dust - a Model Approach.

ROBERT WAGNER, Kerstin Schepanski, Michael Jähn, *Leibniz Institute for Tropospheric Research*

Wildfires, like biomass burning, are a very common phenomenon in semi-arid regions nearly all over the world. Investigations of smoke plumes originating from such wildfires found significant fractions of mineral dust and crust-related minerals within these plumes – raised by strong turbulent winds related to the fire. Since wildfires are not considered as a source of mineral dust in aerosol models so far, a better understanding of the processes, which drive fire-related dust emission, is required.

Therefore, high resolved Large-Eddy Simulations (LES) with the All Scale Atmospheric Model (ASAM) were performed to investigate the impacts of wildfires on the near-surface wind pattern. The analysis of fire-related wind pattern is crucial since the emission of mineral dust is a threshold problem, which means that an efficient mobilization of mineral dust particles requires wind velocities above a certain threshold. The influence of different fire properties (intensity, size, and shape) and different atmospheric wind regimes on the dust emission potential is investigated.

The wind fields derived from the LES fire simulations were coupled with an offline dust emission model to calculate the emission fluxes in dependency on the fire properties and the ambient atmospheric conditions. The gained results can be used to estimate typical values of the emitted amount of mineral dust during wildfires, which can be applied for the development of a parameterization of fire-driven dust emission. With that, an estimation of the importance of the process on a continental scale in relation to other types of mineral dust emissions is possible.

4AM.8

Predicting Atmospheric Gaseous and Particulate Phase PCDD/F Concentrations Using PM2.5 Data and Gas-Particle Partitioning Models of PCDD/Fs. Rong Zhao, Kangping Cui, Weiwei Wang, Lin-Chi Wang, Ping Yan, WEN-JHY LEE, *National Cheng Kung University*

In this study, the data of PM2.5 in Handan City and Kaifeng City, China from 2015 to 2017 were obtained from Environmental Monitoring Website. The total PCDD/Fs-WHO2005-TEQ concentrations in ambient air were predicted by using two established equations for proportional relationships between PM10 and PCDD/F mass concentrations. The obtained total PCDD/Fs-WHO2005-TEQ concentrations in Handan city in spring, summer, autumn and winter were 0.100, 0.058, 0.087, and 0.127 pg WHO2005-TEQ m–3, respectively. The averaged total PCDD/Fs-WHO2005-TEQ concentration in Handan (0.093 pg-WHO2005-TEQ m–3) was 1.3 times of magnitude higher than that in Kaifeng (0.073 pg-WHO2005-TEQ m–3) due to higher consumption of heating coal and atmospheric inversion in winter. Furthermore, AQI index could be used to predict the level of total PCDD/Fs-WHO2005-TEQ in ambient air through regression equation. The R2 in 2015, 2016 and 2017 were 0.929, 0.921 and 0.876, respectively.

4AM.9

Taylor-series Expansion Method of Moments for Resolving Aerosol Dynamics. MINGZHOU YU, Yueyan Liu, *China Jiliang University*

The study on aerosol dynamics processes, such as formation of nano/microscale aerosol particle and its subsequent growth in quiescent or evolving flows, has received much attention from both chemical engineering and atmospheric environment communities[1]. The suitable theoretical method for resolving aerosol dynamical processes is widely known as population balance modelling (PBM), which is on basis of solving the population balance equation (PBE) in terms of particle number concentration. The study on the solution of the PBE has undergone rapid development in last several decades. In this talk, the development of methods of moments for resolving aerosol dynamics widely used in the community of air environment, especially the Taylor-series expansion method of moments will be reported; the emphasis will be placed on the optimization of type of moment sequence, selection of Taylor series expansion point, optimization of an order of Taylor series expansion, and selection of terms for Taylor series expansion of the Taylor-series expansion method of moments[2-6].

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4AM.10

Towards a Coarse-Grained Model of Nano-Particle Agglomeration. MILENA SMILJANIC, Andreas Kronenburg, Rudolf Weeber, Christian Holm, *University of Stuttgart*

The agglomeration of nano-particles plays an important role in many industrial applications, such as particle flame synthesis and spray-drying, where the structure of the agglomerates strongly affects final product characteristics. The process itself consists of two steps: (1) nano-particles collide due to their relative velocities caused by Brownian motion and/or turbulent flow, and (2) they adhere and form aggregates. Detailed models use Langevin Dynamics to track the movement of each particle and compute particle collisions and particle-particle interactions individually, as it is reported in the literature. More recent work investigates the influence of turbulent motion on aggregates' growth and the resulting aggregate morphology. Numerical simulations were, however, limited to rather low numbers of particles (up to 4 million particles) and rather dense particle loadings. This limited the statistics and prevented long simulation times.

The simulation of larger systems will require some simplifications of the modeling process. Here, we develop a coarse-graining approach for the agglomeration of nano-particles and clusters, covering both primary particles of the size of few nanometers to agglomerates that are several orders of magnitude larger. Coarse-graining involves the replacement of parts of the clusters by "representative" particles of (representative) spherical shape. Due to the sparse nature of agglomerates, two spheres that envelop their respective agglomerates could intersect, but the agglomerates that they represent would not necessarily touch and stick. This approach allows not only for collisions on the surface, but also for the particle-cluster or cluster-cluster penetration, based on the calculated collision probability as a function of compactness of the underlying aggregates and of the overlap of the two coarsened spherical particles.

For the calculation of collision probability functions, besides usual agglomerate's morphology characteristics such as number of particles (N), radius of gyration (R_g) and fractal dimension (D_f), we additionally used agglomerate's maximum radius (R_{max}). Assuming random aggregate orientation, we introduce a model of concentric spherical shells, placed at the aggregate's center of mass, with minimal shell radius and shell width equal to the single particle diameter and the maximum shell radius equal to the aggregates maximum radius, respectively. Identical clusters randomly rotated are then shot towards the aggregate, and collisions between their respective particles are saved as hits (n_{hit}) for the corresponding cluster shells. On the contrary, penetration of the tested clusters through shells without detecting any collision are accounted for misses (n_{miss}). For each cluster there are conducted N=3000 simulations and averaged within several cluster groups, over 100 clusters for each cluster group. This study examines aggregates of following characteristics: Rg=(3,5,7) and Df=(1.6,2.0,2.4).

Distance dependent collision probabilities ($P_{coll,i}$) have been calculated as

$P_{coll,i}=n_{hit,i/}(n_{miss,i}+n_{hit,i})$.

As results show, along the interaction radius collision probability function is strongly affected by the aggregate fractal dimension and radius of gyration, slightly varying within relatively confined parameter ranges. In addition to it, results on cluster-cluster collision probabilities are used in coarse-grained simulations as determining parameter for creating bonds between colliding coarsened particles and their further growth, as well as for modelling of cluster-cluster interactions.

4AM.11

High Resolution Chemical Transport Modeling of Ultrafine Particles over Pittsburgh. SHAYAK SENGUPTA, Pablo Garcia, David Patoulias, Provat Saha, Wei Ma, Christopher Tessum, Iannis Kioutsioukis, Sean Qian, Spyros Pandis, Inês Azevedo, Peter Adams, *Carnegie Mellon University*

Ambient ultrafine particles (UFPs), solid or liquid particles in the atmosphere with diameters less than 100 nm, pose poorly understood human health impacts relative to well-understood impacts of $PM_{2.5}$. Numerous studies have documented health effects related to roadway proximity, with UFP emissions from traffic as a possible culprit. However, high spatial variability and the lack of widespread monitoring complicate exposure quantification of UFPs. The goal of this work is to develop and evaluate high resolution (1 km) chemical transport model (CTM) simulations to quantify UFP concentrations as a step towards quantifying UFP exposure in an urban area. This study uses PM-CAMx-UF to predict UFP concentrations in the Pittsburgh metropolitan area at 1 km spatial resolution for multiple seasons in 2016 and 2017. PM-CAMx-UF is a state-of-the-science CTM which simulates the production and destruction of UFPs in the atmosphere by explicitly tracking both particle number and mass concentrations. Model inputs include traffic emissions at 1 km resolution, spatially resolved using a traffic model for Pittsburgh. Simulations test the CTM's ability to accurately predict UFP concentrations and understand which sources impact particle number concentrations. Furthermore, we test simulations at 4 km, 12 km and 36 km resolutions to identify and compare the amount of spatial variability in UFP concentrations resolved by the CTM. We evaluate our model predictions with a distributed, intraurban network of observation sites which includes stationary water-based condensation particle counters, scanning mobility particle sizers, and beta attenuation monitors to monitor both particle mass and number concentrations in traffic-heavy and non-traffic-heavy locations. Mobile van sampling throughout Pittsburgh complement stationary observations to evaluate model performance. In addition to showing model performance evaluation, use of model results to predict population exposure will show the impact of model resolution on quantifying UFP and PM2.5 exposure. Any nonzero correlation between predicted total particle number concentration and $PM_{2.5}$ mass concentration suggests potential exposure confounding in long-term health impact quantifications.

4AM.12

Simulation of SOA Formation of Monoalkyl-substituted Benzenes in the Presence of SO2 under Different NOx Levels Using the UNIPAR Model.

CHUFAN ZHOU, Myoseon Jang, *University of Florida*

The secondary organic aerosol (SOA) formation from the photooxidation of hydrocarbons is influenced by the concentration of coexisting tracers such as NOx and SO2, the meteorological conditions (humidity and temperature), and atmospheric aging. SOA contributes significantly to total fine particulate matter, and yet the prediction of SOA formation remains inadequate. Our laboratory's recent research efforts have improved the state-of-the science-art via the development of the Unified Partitioning-Aerosol Phase Reaction model (UNIPAR), which utilizes explicit gas chemistry to predict SOA formation from multiphase reactions. The UNIPAR model vastly improved the accuracy of chamber generated SOA mass predictions. The oxidized semivolatile organic compounds predicted using gas-phase explicit mechanisms are lumped into 8-volatility. Each volatility group is further classified into 6-groups based on their emerging chemistry in the aerosol phase. Glyoxal (Gly), methylglyoxal (MGly), and IEPOX are separately treated in UNIPAR because they are known to significantly contribute to SOA formation. The UNIPAR model features the dynamic product stoichiometric coefficients (51 lumping groups) that can change with atmospheric aging and NOx levels. Additionally, thermodynamic parameters (activity coefficients of lumping groups) in the model are also dependent of the aging process and NOx levels. The impact of the aging process on the model parameters was dynamically treated using the quantity of typical radical species (i.e., HO2 and RO2), which are commonly predicted in most chemical mechanisms in air quality models. Among urban hydrocarbons, monoalkyl-substituted benzene are important precursors to form SOA. In this study, the feasibility of the UNIPAR model is demonstrated to SOA formation from various monoalkyl substituted aromatic SOA against chamber data from University of Florida Atmospheric Photochemical Outdoor Reactor (UF-APHOR). The lumping base UNIPAR, constructed using explicit mechanism, enables the flexible treatment of multiphase partitioning and aerosol chemistry (i.e. oligomerization in organic phase, acid-catalyzed reactions in inorganic aqueous phase, and OS formation). As a result, UNIPAR is able to improve the ability to accurately estimate SOA mass, which is under-predicted by current regional models.

4AM.13

Effect of Dispersion & Coagulation Parameters on the Survival Fraction of Aerosol Particles Released from Puffs and Plumes.

Tanmay Sarkar, S. Anand, Y.S. MAYYA, *BARC*

The concept of particle survival fraction finds important application for estimating the contribution of localized emission sources to the persisting aerosol background in the atmosphere. In recent times, this concept has found an important application in the area of geo-engineering proposals in order to slow down global warming, in which light scattering aerosol plumes are supposed to be deliberately released from ships to the clouds to enhance marine cloud brightening. As the particles releases from highly inhomogeneous sources, they would undergo significant coagulation during their dispersal to form background aerosols. An effective way of quantifying this effect is to model their survival fraction by combining coagulation equation with dispersion equation. A major difficulty arises while combining aerosol microphysical processes with dispersion equation, particularly coagulation process as it leads to non-linear integro-differential equation. Several approaches have been developed by various authors in the past to solve the governing equation for particles undergoing simultaneous dispersion/Brownian diffusion and coagulation, such as analytical solutions to special cases (Simons, 1996), expanding plume models (Turco and Yu, 1999). The diffusion–coagulation equation that governs the evolution of a spatially inhomogeneous aerosol puff and plumes is solved by Anand and Mayya (2011). This model is extended to geo-engineering problems (Anand and Mayya, 2015). To make the solution methods or numerical computations simpler, several approximations on 1) particle size distribution, 2) coagulation kernel, and 3) dispersion process are made.

In the present study, we examine the effect of these parameters on the survival fraction of particles in a spherical puff through exact numerical calculations. The numerical program can consider any initial particle size distribution such as lognormal, exponential, etc., and coagulation kernels such as free-molecular and Fuchs kernels, which can handle fractals also. The diffusion coefficients for the particles released from the point sources are generally expressed as either space- or time-dependent variables. The study demonstrates that the survival fraction will be lower for an initial polydisperse spectrum as compared to a mono-disperse spectrum. The effect of polydispersity is further studied by varying the parameters of initial size distribution (CMD and GSD). The inclusion of Fuchs kernel and non-constant dispersion coefficient in the numerical program affects the evolution of particle survival fraction compared to the constant kernel case. These realistic simulations finally determine the fraction of emitted particles survived due to combined action of coagulation and atmospheric dispersion. This model is proposed to compute source emission correction factor for various indoor emission sources to estimate effective number concentration to the indoor background environment and then to global aerosol background.

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4AM.15

Aerosol Impaction under High Knudsen Number, High Mach Number Conditions for Applications in Additive Manufacturing.

CHENXI LI, Bernard Olson, Christopher Hogan Jr., *University of Minnesota*

Aerosol deposition has emerged as a novel additive manufacturing (AM) method for surface coating and thin film production. Though inertial impaction is typically the deposition mechanism, AM based deposition functions in a very different regime from traditional sampling based impactors. Specifically, the AM process involves accelerating supermicrometer particles (rarely submicrometer particles) with a high-speed carrier gas leading to particle at supersonic speeds with the potential plastic particle deformation on the substrate. It is generally acknowledged that the instantaneous particle speed upon impaction is critical to controlling coating/film properties such as porosity, and mitigating particle bounce during deposition. Therefore, to achieve desirable particle impaction speed, converging-diverging nozzles (i.e. de Laval nozzles) are frequently used to accelerate particles.

Though considerable effort has been devoted to simulation of particle trajectories as well as impaction speed, some critical aspects of using de Laval nozzles for particle acceleration are yet to be fully understood. This presentation discusses two issues related to this process. The first issue concerns drag force exerted on particles by carrier gas. As particles traverse through the nozzle, rapid gas rarefication and densification (due to a shock) can lead to particle Knudsen number (Kn) variations by as much as ~100, ranging from the free molecular to continuum regimes. In addition, due to gas stagnation close to substrate or insufficient particle acceleration, particle Mach numbers (Ma, based on relative speed of gas and particles) can exceed unity with potential shockwave formation close to the particle surface. Simulation of particle trajectories, therefore, requires a drag law that is valid for a wide range of of Kn and Ma. The first part of this presentation consists of summary and comparison of the existing drag laws with a focus on range of validity, and proposal of a new drag law based on direct simulation Monte Carlo valid for the range $0 < Kn < \infty$ and $0 < Ma < 3$.

The second issue relates to how operating conditions of the converging/diverging nozzle influences particle impaction speed. Specifically, two factors are discussed: (1) particle size, (2) upstream/downstream pressure of the nozzle. Given other operating conditions, we show that impaction speed is a function of particle size, with an optimum particle size with the maximum impaction speed for a given nozzle geometry. As to upstream/downstream pressure, our simulations demonstrate they change the shock wave structure and have a significant effect on deceleration of nanosize particles by changing the gas pressure close to the substrate.

4AM.17

Quantifying and Valuing the Role of UK Vegetation in the Removal of Particulate Matter. EIKO NEMITZ, Laurence Jones, Massimo Vieno, Daniel Morton, Carnell Ed, Stefan Reis, Ian Dickie, Philip Cryle, Holland Mike, *Centre for Ecology and Hydrology*

Air pollution presents a major risk to human health, resulting in premature deaths and reduced quality of life. Vegetation can play a role in reducing concentrations of air pollutants, but estimates of the service that vegetation provides are highly variable.

The majority of methods used to calculate pollution removal are driven with static concentrations and therefore ignore the feedback of removal on concentrations, and interactions with wet deposition processes and between compounds.

In this study we applied an atmospheric chemistry and transport model (EMEP4UK) to calculate the amount of pollutant removal in the UK by current vegetation for $PM_{2.5}$, but also gaseous pollutants (NO_2, NH_3, SO_2, O_3) by comparing a model run with current landcover to a baseline scenario in which vegetation was replaced by bare soil. From these data we calculated the health benefits from the changes in pollutant concentrations (i.e. change in exposure) induced by the additional pollution removal by the vegetation.

Results show that current UK vegetation as a whole reduces concentrations of $PM_{2.5}$ by around 10%, far greater than in previous studies. The economic value of the health benefits are substantial: £1 billion in avoided health costs estimated for 2015, resulting from 1900 avoided deaths, 27,000 avoided life years lost, 5,800 fewer respiratory hospital admissions and 1,300 fewer cardiovascular hospital admissions.

We also show that the benefits do not always occur in the same location as the pollutant removal. In other words the benefits, defined in terms of reduced pollutant concentrations, are also transported in the atmosphere.

4AM.18

Prediction of the Chamber Wall Process of Gaseous Semivolatile Organic Compounds Using a Linear Solvation Energy Relationship. HUANHUAN JIANG, Myoseon Jang, Sanhee Han, *University of Florida*

The chamber wall process of gaseous and semivolatile organic compounds has been known to significantly influence studies of secondary organic aerosol (SOA) formation. For example, the wall process of gaseous semivolatile organic compounds leads considerable underestimation of SOA yields (e.g., 30% for toluene SOA) and furthermore affects the credibility of the predictive SOA model derived using chamber data. In this study, a mathematical model is built to predict the of uptake coefficient of a gaseous semivolatile organic compound by the integration of the deposition kinetics of organic compounds with a Linear Solvation Energy Relationship (LSER). The deposition process of organic compounds is approached using a conservation balance via on- (adsorption) and off-kinetic mechanism (desorption) between the gaseous phase and the chamber wall phase. The adsorption rate constant (k_{on}) of organic compounds is processed using a conventional mass transfer process. The desorption rate constant (k_{off}), which is linked to both an off-gassing rate constant and the gas-wall partitioning coefficient of an organic compound, *i*, ($K_{\mathrm{i,wall}}$), is semiempirically predicted by fitting the measured decay rate of compound *i* to the thermodynamic physicochemical parameters based on LSER. Various model compounds (i.e., long-chain deuterated alkanes, alcohols, carboxylic acids, and carbonyls, substituted phenols) are introduced into the large outdoor smog reactor (UF-APHOR chamber). The deposition rate constants of these compounds are measured using the traditional denuder sampling integrated with a gas chromatography-mass spectrometer (GCMS) in the course of a 12-hour wall-loss process. The resulting deposition rate constants are applied to the derivation of the model. Our recent exploratory data proved that the deposition process was well-predicted using the newly derived LSER base model. In this study, the resulting wall process model will be applied to the estimation of SOA yields and improve the quality of explicit SOA models (i.e., UNIPAR).

4AM.19

3-D Numerical Study of Linear Slot Virtual Impactor. WONYOUNG JEON, Hyunwoo Lee, Youngjin Seo, *Kumoh National Institute of Technology*

Virtual Impactor (VI) is used to classify particles into two sizes or to concentrate them to increase the concentration of particles. The basic principle of VI is to take advantage of the inertia that particles get through the accelerating nozzle. The most important point when designing a VI is to minimize the loss of particles (deposition due to collisions with walls). Losses at the wall has an adverse effect on VI performance. This study focuses on developing and optimizing the VI that operates at the flow-rate of 150 LPM. Target cut-point is 1 micrometer. The research is conducted for three steps. First, we numerically optimize the 2-D LSVI (Linear Slot Virtual Impactor). Second, we characterize 3-D geometry by simulating 3-D LSVI by selecting several revamped 2-D models. The particle simulation for the 3-D LSVI will be carried out at particle diameters in the size range of 0.1 to 15 micrometers. Finally, experiments will be conducted to verify the optimization model using fluorescent particles (0.3 to 10 micrometers). Experiments will be conducted in a closed-loop system. In this paper, we present how the critical geometry factors change the performance of a VI through 3-D simulation. In addition, we will present preliminary experimental data out of the 3-D model.

4AM.20

Numerical Investigation on Artificial Cloud Seeding as a Means of Precipitation Enhancement. ALI AFZALIFAR, Juha Tonttila, Kudzotsa Kudzotsa, Tomi Raatikainen, Harri Kokkola, Sami Romakkaniemi, *Finnish Meteorological Institute*

Globally, about 1.2 billion people lack access to water and more than twice this number suffer from inadequate sanitation and seasonal water scarcity. Given the present consumption rate of water, this problem will only become worse. Cloud seeding, in form of artificial emission of large particles from ground or a flying aircraft, is thought to provide a promising solution to this problem particularly in regions with low rainfall. Over the years, although several studies have corroborated the positive correlation between the cloud condensation nuclei, emitted through cloud seeding, and precipitation formation, the confidence in the effectiveness of cloud seeding is still far from absolute. In the present work, the large eddy model UCLALES along with the aerosol module SALSA is applied to study aerosol-cloud microphysical processes at a cloud-resolving scale. The model UCLALES-SALSA employs a detailed sectional microphysical scheme which represents the size distribution of aerosol, clouds and precipitation in terms of number of fixed size sections. The latest version of the model benefits from schemes for both natural and artificial aerosols emissions, thus it provides a powerful means to predict the effects of cloud seeding on precipitation. Moreover, the experimental study on the effects of artificial emission of giant cloud condensation nuclei on precipitation, performed by Jung et al. (2015; ACP), is used to validate the modelling results in this work.

4AM.21

A Simulation Tool to Understand the Chemistry of Hexavalent Chromium in Airborne PM at pH 5 and pH9. MEHDI AMOUEI TORKMAHALLEH, Dinara Konakbayeva, Marios Fyrillas, Mirat Karibayev, *Chemical and Aerosol Research Team, Nazarbayev University*

Chromium is found in the atmosphere in two stable oxidation states, trivalent chromium (Cr(III)) and hexavalent chromium (Cr(VI)). Cr(III) is an essential element for living organisms, mainly involved in the control of lipid and glucose metabolism. Conversely, Cr(VI) is a toxic element, and based on the exposure duration it causes adverse health effects such as perforation of the nasal septum, asthma, bronchitis, pneumonitis and lung cancer. Insoluble forms of Cr(VI) might be more toxic than soluble compounds. Soluble Cr can enter the blood and be excreted or be converted to Cr(III) in the blood stream. Animal studies demonstrated that slightly soluble and highly insoluble Cr(VI) particles such as the chromates of zinc, lead, strontium, barium, and sintered calcium consistently induced a tumor response, albeit with variable efficacy. Thus, it is imperative to investigate the soluble and insoluble fractions of Cr in the atmosphere to better understand its health effects. To obtain a more complete picture of atmospheric aqueous Cr speciation, Cr chemistry in the presence of a mixture of atmospheric oxidants and reductants including ambient PM matrix and dissolved gases needs to be investigated. Nevertheless, soluble and insoluble forms of the Cr(III) and Cr(VI) were not investigated in previous modeling studies. Currently, Cr(VI) sampling involves collecting PM on a filter at pH 9 and is integrated with wet chemical analysis. PM on the sampled filters is extracted using an alkaline or acidic solution that is then analyzed by Ion Chromatography (IC) or a combination of IC and ICPMS, respectively. However, wet analysis procedures may not extract the insoluble Cr(VI) and thus, may underestimate atmospheric Cr(VI) concentrations. Understanding the soluble and insoluble forms of Cr in the atmosphere using modeling studies will assist in better designing and integrating Cr(VI) sampling and analysis systems. The objective of this study was to develop a conceptual model for the aqueous chemistry of the atmospheric Cr where Cr is a non-limiting reactant, and to implement this model to better understand the soluble and insoluble forms of Cr(III) and Cr(VI) compounds under atmospheric and sampling conditions. This model is also applicable to locations where Cr emitting industries exist. The results of the present investigation will be helpful in developing an analytical method to quantify total Cr (soluble and insoluble) species in the atmospheric PM. Field measured concentrations of atmospheric species were utilized as model input in this study. The dominant form of Cr(VI) in the pH 5 solution was found to be Cr2O7 2-. At pH 5 chromate was produced by the dissolution of Na2CrO4(s) and K2CrO4(s) available in the solid core, but a considerable portion of the CrO4 2- precipitated as (NH4)2CrO4(s), CaCrO4(s), BaCrO4(s) and PbCrO4(s). Cr(OH)3 was found to be soluble, and the insoluble form of Cr(III) was Cr2(SO4)3. Conversion of Cr(VI) to Cr(III) was higher than the conversion of Cr(III) to Cr(VI). The simulation results agree with the field measurements near Cr industries. At pH 9, CrO4 2- was the dominant soluble form of Cr on the sampling filter while (NH4)2CrO4, CaCrO3, BaCrO4, PbCrO4 were the dominant form of insoluble Cr(VI). Reduction of Cr (VI) to Cr (III) was higher than the oxidation of Cr (III) to Cr (VI).

4AM.23

Evolution of PM Components in Europe over the 1990-2010 Period in the Framework of the Eurodelta-Trends Exercise. GIANCARLO CIARELLI, Augustin Colette, Matthias Beekmann, Mark Theobald, Peter Wind, Camilla Andersson, Florian Couvidat, Astrid Manders-Groot, Mihaela Mircea, Maria Teresa Pay, Valentin Raffort, Svetlana Tsyro, Kees Cuvelier, Mario Adani, Bertrand Bessagnet, Robert Bergstrom, Gino Briganti, Andrea Cappelletti, Massimo D'isidoro, Hilde Fagerli, Yelva Roustan, Marta Vivanco, *LISA*

Recent studies have investigated the changes in particulate matter (PM) concentrations over the past decades in Europe. However, only a few have investigated the evolution of the individual PM components, i.e. inorganic and organic phases, following the implementation of emission reduction strategies. The trends in PM components might differ as a result of the different chemical regimes in different European regions and the non-linear response of PM to changes in precursor emissions. Thus, understanding how the chemical composition of PM has varied during the last decades could provide more insight for future air quality legislation.

In the framework of the EURODELTA-Trends (EDT) modeling exercise, several Chemical Transport Models (CTMs) were applied for the 1990–2010 period in order to investigate air quality changes in Europe due to the implementation of emission reduction strategies. A common anthropogenic emission dataset was used by the modeling teams (i.e. NO_2, SO_2, HN_3 and non-methane VOCs) based on estimates from the Greenhouse gases and Air pollution Interactions and Synergies (GAINS) model. Model simulations were conducted at 0.25° and 0.4° resolution in latitude and longitude, respectively, with a domain extent from 17° W to 39.8° E and from 32° S to 70° N. Five CTMs have provided air quality estimates for a 21 year period (i.e. CHIMERE, EMEP/MSC-W , MATCH, LOTOS-EUROS and MINNI).

For this study, we combined consolidated long-term air quality measurements of sulfate (SO_4^{2-}), total nitrate (TNO3), total ammonium (TNH4), as well as sulfur dioxide (SO_2) and nitrogen dioxide (NO_2) available for multiple sites in Europe for the 1990–2010 period with output data from the CTMs used in the EDT exercise.

Comparisons between modeled and measured data showed a relatively good agreement between the model ensemble and the measured data. In particular, the faster decline in SO_2 and SO_4^{2-} concentrations in the first decade analyzed (1990–2000) compared with the second one (2000–2010) was well captured by the model ensemble. For TNO3 and TNH4 concentrations, both the measurements and the model ensemble showed rather flat trends for both periods, with larger differences in trend significance occurring at a single station level. The evolution of the modeled secondary organic aerosol (SOA) concentrations were also investigated together with the trends in emissions of biogenic volatile organic compound (VOCs). For the models that provided biogenic emission data, a statistically significant increase in biogenic emissions (i.e. isoprene and monoterpene) was found along with an increase in the relative contribution of biogenic SOA (B-SOA) to the total SOA.

In addition, modeled SOA concentrations were evaluated against positive matrix factorization (PMF) data available during the second decade. Results indicated a systematic under-estimation of the modeled SOA fraction with large differences between the models, most likely due to the different levels of complexity of the SOA schemes.

4AM.24

Comprehensive Organic Emission Profiles for Mobile Sources: Integration of VOC, IVOC, SVOC and Lower Volatility Organics.

QUANYANG LU, Yunliang Zhao, Albert Presto, Andrew May, Tim Gordon, Allen Robinson, *Carnegie Mellon University*

Mobile sources contribute about one-third of anthropogenic organic emissions in the 2014 EPA National Emission Inventory (NEI); they are an important source of POA (primary organic aerosol) and SOA (secondary organic aerosol) precursor gases, especially in urban environments. Traditional emissions inventories account for two types of organics: volatile organic compounds (VOCs) in the gas-phase and particulate matter (PM). However, this is an overly simplistic representation.

We compiled recently published data to create comprehensive model-ready organic emission profiles for gasoline, gas-turbine, and diesel sources. Our source profiles span the entire volatility range, from nonvolatile organic compounds (NVOC) to low-volatile organic compounds (LVOC), semi-volatile organic compounds (SVOC), intermediate-volatile organic compounds (IVOC) and VOC. The overall mass closure of integrated organics to bulk measurement of non-methane organic gases and organic carbon (NMOG+1.2*OC) is 0.83 for on-road gasoline source, and ~1 for on-road diesel source.

The fractions of IVOC and SVOC to the total organic emissions (NMOG+1.2*OC) are consistent within source type: contributing about 4.5% (2.4%-9.6% as 10th to 90th percentile) and 1.1% (0.4%-3.8%) for gasoline engines, 20-27% and 4.5-7.5% for gas-turbine engine, and 52.5% (45.5%-60.0%) and 4.0% (3.0%-4.6%) for diesel engines.

Organic emissions from all source categories have tri-modal volatility distributions. The largest model is ‘fuel’ mode, which contributes 72.6% (66.5%-77.6%) total organic emissions in gasoline, 65.2% (59.8%-79.6%) in diesel exhaust, and 37.5-38.5% for gas-turbine. The ‘fuel’ mode mirrors the trends in fuel volatility. Emissions from each source also has a low-volatility mode, comprised of SVOCs and even less volatile organics, which peaks at a C* of 10 $\mu g\ m^{-3}$. The final mode is the most volatile, peaking at a C* of 10^{10} or 10^{11} $\mu g\ m^{-3}$. It contributes about 25% of the total organics in gasoline and diesel exhaust, and 50-57% for gas-turbine engine exhaust. The composition of this mode is primarily comprised of alkenes and carbonyls.

IVOCs are enriched in the exhaust relative to the fuel, especially for gasoline sources. Sources using more volatile fuel have higher IVOC enrichment factors. Gasoline engine exhaust has a median enrichment factor of 8.5 versus no enrichment for diesel exhaust. Gas turbine exhaust falls in between.

Three approaches are used to parameterize IVOC emission for use in SOA models, which are 1-group, 4-group and source-specific parameterizations. First, using a single lumped group for all sources, we obtained the relative error is ≤20% for gasoline and diesel source, and ≤40% for gas-turbine source, within OA concentration from 0 to 20 $\mu g\ m^{-3}$. Second, when using 4-group parameterization, the relative error is reduced to ≤15% for gasoline and diesel source, and ≤35% for gas-turbine source. Third, by fitting for each source separately, relative error for all sources could be bounded within 10%.

The new profiles predict that IVOCs and SVOC vapors contribute significantly to SOA production, especially for sources using lower volatility fuels. For gasoline sources, IVOCs and SVOC vapors contribute ~80% SOA than tradition VOC precursors. For gas-turbine and diesel sources, IVOCs and SVOC vapors contributions exceeds the SOA production from VOC emissions by a factor of 18 and 38, respectively. Also, the new profiles treat POA as semi-volatile, and they predict that 40%-50% of POA mass evaporates at ambient conditions. There is a large change in the composition of the OA, changing from 50% (traditional) to more than 80% (new) of gasoline OA mass is SOA.

4AM.27

Urban Air Quality Modeling at High Spatial Resolutions. PABLO GARCIA, Peter Adams, Spyros Pandis, *Carnegie Mellon University*

Human activities in dense urban areas produce significant emissions of atmospheric pollutants and their precursors and these have adverse health effects on the exposed population. Emission sources like traffic and restaurants have significant variations at the urban scale. Resolving the pollutant concentration fields and the health impacts associated with these and other sources requires emission inventories, measurements and simulations to be available at high resolutions. A high resolution emission inventory was developed for the city of Pittsburgh and surrounding counties based on the EPA's National Emission Inventory (NEI) for 2011 with novel spatial surrogates to geographically distribute emissions in a grid of 1x1 km cells. This inventory was used to predict gaseous pollutants and speciated particle matter (PM) concentrations with the PMCAMx chemical transport model for the period of the Center for Air, Climate and Energy Solutions (CACES) campaign in Pittsburgh. Model predictions were compared with national speciated PM networks and Aerosol Mass Spectrometer data from the CACES supersite. The predictions were also compared with measurements taken with a mobile laboratory at high spatiotemporal resolution in urban and suburban areas in Pittsburgh. These comparisons were repeated with a baseline simulation using the standard NEI approach. PMCAMx predicts concentrations reasonably well, showing improvement when compared to the standard NEI approach.

4AM.28

Coupled Gas and Particle Phase Modeling of Isoprene SOA Formation. KELVIN BATES, Rebecca Schwantes, John Seinfeld, *California Institute of Technology*

Following the creation of a state-of-science gas-phase isoprene oxidation mechanism, a new module has been developed to simulate secondary organic aerosol (SOA) formation from isoprene oxidation under a wide range of conditions by coupling a reduced version of the gas-phase mechanism to a simplified particle-phase mechanism. The model is prepared in Kinetic PreProcessor (KPP) format for easy simulation of environmental chamber experiments. We present results from a series of simulations of experiments performed in the Caltech environmental chambers investigating SOA yields directly from OH-initiated isoprene and methacrolein oxidation under various [NO], [NO_2], temperature, humidity, and seed aerosol conditions. Both the model and the experiments incorporate SOA formation from isoprene epoxydiols (IEPOX), methacryloyl peroxynitrate (MPAN), and highly functionalized semi-volatile isoprene derivatives. The model code will be made freely available online as part of the existing gas-phase isoprene oxidation mechanism (DOI 10.22002/D1.247).

4AM.29

Modeling the Effects of Central American Fire Emissions on Air Quality in Texas. QIANJIN ZHENG, Min Zhong, *Texas A&M University-Kingsville*

Natural and anthropogenic fires emit the significant number of particles and gaseous air pollutants. Each year during the spring season, large amounts of smoke from the Yucatan Peninsula and southern Mexico transport across the Gulf of Mexico and reach the south-central United States. This long-range transported smoke causes deteriorating air quality periodically in Texas. As anthropogenic emissions continue to decline steadily, the contribution of emissions from long-range smoke will likely increase. This research leverages the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem) to study the impact of fire emissions from Central America on surface fine particle matter ($PM_{2.5}$), aerosol optical depth (AOD), carbon monoxide (CO), and Ozone (O_3) in Texas. The model domain covers multiples states in southern U.S., Mexico, and Central America at 12 km horizontal resolution. The anthropogenic emissions inventory is based on a global emission inventory; the Hemispheric Transport of Air Pollution (HTAP_V2.2) and Fire INventory from NCAR (FINN) is used for fire emissions. The initial and lateral boundary conditions for chemical species are taken from the MOZART global chemical transport model. The gas-phase and aerosol chemistry are represented by the Regional Atmospheric Chemistry Mechanism (RACM) and the Model Aerosol Dynamics for Europe with the Secondary Organic Aerosol Model (MADE/SORGAM), respectively. In-situ ground measurements and satellite observations are applied to evaluate the WRF-Chem model performance in March-May 2013. We find that smoke from Central America spreads across certain areas in Texas and significantly affects the local and regional air quality. Our study indicates that long-range fire emissions should be considered in evaluating the relative effectiveness of local emissions control program.

4AM.30

Climate System Responses to the Interactions between Wildfires and Climate. AOXING ZHANG, Yuhang Wang, Yufei Zou, *Georgia Institute of Technology*

While the effects of climate on wildfires and those of wildfires on climate have been studied in the past, little is known how the feedbacks between wildfires and climate affect the climate system behaviors. For example, large amounts of aerosols released by wildfires change regional climate through direct radiative forcing and aerosol-cloud processes. The resulting regional climate changes also regulate the occurrence frequency, magnitude, and duration of wildfires. Similar interactive processes also take place for fire-induced land surface and vegetation changes. These interactions have not yet been carefully studied because current climate models lack the capability of simulating the interactions between wildfires and climate. We have developed the REgion-Specific ecosystem feedback Fire (RESFire) model and implemented it into the Community Earth System Model (CESM), which allows us to examine the responses of wildfires and climate to their interactions. We find that wildfire-climate interactions due to aerosols tend to decrease the global precipitation, although regional variations in magnitude and sign are large. The western United States, for example, shows a clear drying effect. While the aerosol effects tend to be short-term (days-weeks), the climate responses can be inter-seasonal and interannual. The fire induced land cover changes, the effects of which last much longer (years), also affect the climate system behavior in short term. We examine further the differences of wildfires and climate interactions at present to the future projections based on the RCP4.5 scenario and find that the system responses differ as the climate warms.

4AM.31

Formation of Sulfate during Winter High Pollution Events in Beijing. Peng Wang, Li Wu, QI YING, Jianlin Hu, Hongliang Zhang, *Texas A&M University*

Sulfate is a major aerosol component in severe winter haze events in many areas across China. Debates on the importance of various pathways of S(IV) to S(VI) oxidation, including gas and aqueous reactions as well as heterogeneous reactions have been ongoing without a clear consensus. Recently, the importance of the aqueous phase oxidation by NO2 and by O2 catalyzed by transition metals is being extensively discussed. In this study, we applied a modified CMAQ model to evaluate the contributions of these different pathways to sulfate formation in January 2013 when daily average sulfate concentration reached more than 100 μg m^{-3}. A sulfate formation tracking method based on the source-oriented modeling approach is implemented to track sulfate from different pathways. To have a better understand of the vertical distribution of the sulfate formation rate, the source-oriented approach also keeps track of sulfate formation of different vertical layers. By doing this detailed modeling exercise, we aim to provide more detailed understanding of the sulfate formation processes in the region.

4AM.33

Brownian Diffusion of Nano-Fibers. LIN TIAN, Goodarz Ahmadi, Jiyuan Tu, *RMIT University*

Motion of nanoparticles that are suspended in fluids are dominated by Brownian diffusion – a physical property well understood following Einstein (1905). While theoretical derivation and experimental measurement of the diffusion coefficients for spherical particles are well developed, such information for non-spherical particles are lacking. In this study, the Brownian diffusion of elongated nano-fibers is investigated numerically. Motion of the nano-fiber is resolved by solving the system of equations governing its coupled translational and rotational motion. To isolate the Brownian diffusion from other diffusive forces, test fibers are immersed in an unbounded quiescent fluid where only the hydrodynamic drag and Brownian forces are present. The study allows a close look at the Brownian diffusion of the nano-fibers with respect to the translation, rotation, coupling, and how the rotation affects the particle's macroscopic diffusion properties. Particular attention was given to the rotational relaxation time in determining the non-spherical particle's isotropic and anisotropic diffusive properties. Theoretical and semi-empirical equations are developed to quantify the diffusion coefficients of nano-fibers. The predications are compared with the experimental data, and excellent agreement was obtained. The study opens up new approaches for studying fundamental diffusive processes of nano-particles of complex shapes which are abundant in natural environment.

4AP.1

The Concentrations of Aerosol Surface Area in Fukue Island, Japan, Measured by Diffusion Charging Method. MIHO KIRIYA, Tomoaki Okuda, Ayako Yoshino, Akinori Takami, Indra Chandra, Takafumi Seto, Koji Funato, Kozo Inoue, *Keio University*

Observation of the ambient aerosol surface area concentrations is important to understand the aerosol toxicity because an increased surface area may be able to act as an enhanced reaction interface for certain reactions between aerosol particles and biological cells, as well as an augmented carrier surface for co-pollutants. In this study, the aerosol surface area concentration was measured together with black carbon (BC) and other chemical species such as organic compounds, sulfate, and nitrate on April 2017 in Fukue Island, Japan. The concentrations of aerosol surface area were highly correlated with those of BC, which has relatively large surface area since BC particles are usually submicron agglomerates consisting of much smaller (tens of nanometers) sized primary soot particles. Compared with the concentrations of aerosol surface area in Fukuoka city, those in Fukue Island did not increase at daytime. This was due to low BC concentrations because of small traffic volume in suburban area of Fukue Island. Also, there were some cases which the concentrations of aerosol surface area did not increase even though sulfate concentrations increased. According to the airmass backward trajectories analysis, those low surface area-high sulfate events seemed to be affected by the airmass from East China Sea.

4AP.2

Measurement of the Electrostatic Charging State of Ambient Aerosol Using a Parallel Electrode Plate Device. KENTARO FUJIOKA, Keiichi Kurosowa, Takuto Yonemichi, Koji Fukagata, Tomoaki Okuda, *Keio University*

In recent years, the influence on health by fine aerosol particles such as PM2.5 has been concerned. Especially regarding the particle deposition in a human airway, some previous researches showed that charged particles were deposited to airway surface several times as much as uncharged particles. In other words, when we inhale an aerosol particle, it is deposited on the airway more than expected from its particle size if the particles are charged. However, little knowledge on the electrostatic charging state of atmospheric aerosols has been obtained so far. Therefore, in this study, we measured the charging state of atmospheric aerosols from April 2017 using a parallel electrode plate device utilizing the principle of electric mobility. The results varied depending on the measurement day, and the proportion of charged particles was about 75~88%. By investigating the relationship between the charging state and the weather condition at the time of measurement, it was found that there was a strong positive correlation between the proportion of charged particles and the absolute humidity.

4AP.4

Dynamics of Molecular Ions under the Electrical Field. TOMOYA TAMADATE, Takaaki Orii, Hidenori Higashi, Mikio Kumita, Yoshio Otani, Takafumi Seto, *Kanazawa University*

Highly charged macromolecular ions exhibit various conformations in the gas phase. Intramolecular charge-to-charge interactions induce the transition from the globular structure into the stretched conformation (Larriba and de la Mora, 2012). Such variation of molecular conformation causes complex gas phase dynamics of ions under the electrostatic field. In the present study, the dynamics of multiply-charged molecular clusters were visualized by molecular dynamics (MD) simulation.

The MD simulation was performed by the system consisting of one molecular ion (PEG or tetra-alkyl ammonium ion) with 200 N_2 molecules located in a cubic simulation cell (L=20 nm). The temperature was set at 298 K. In order to simulate the electrical drift of the molecules, the electrical field was applied as $E_x = E_y = E_z = 10{,}000\ \mathrm{V\ cm^{-1}}$.

From the results of visualization by the simulation, the conformation of multiply charged PEG molecules in the gas phase changed from sphere to the non-spherical (string shape) due to the repulsive force between partial charges on the molecule. Such structural transition depends on the number of charges and molecular weight of PEG. In addition, the orientations of the highly charged PEG molecules varied under the electric field. Therefore the transport properties of the highly charged ions were influenced by the molecular structure, charge localization, and orientation.

The electrical mobility of molecular ions was calculated from the change in the position during the specific time interval. Firstly, the MD-calculated mobility of the spherical molecules was validated by the comparison with theoretical values obtained by the Stokes-Einstein's equation. Then, the electrical mobility of the PEG molecules was calculated by the MD simulation with changing molecular weight and the number of charges. It was found that the change in the conformation of the PEG molecules caused a decrease in the calculated mobility, which was also reported in the literature. Thus, the MD simulation is considered to be an effective tool to estimate the electrical mobility of the highly charged macromolecules.

4AP.5

Effects of Dehydration Conditions on Particle Morphology and Activation Ratio of Inorganic Nanoparticles by a HT-DMA- APM / CCNC System.

TA-CHIH HSIAO, Po-Hsiang Huang, *National Central University*

Morphology of aerosol particles may play an important role in pharmaceuticals, powder industry, and atmospheric science. Numerous literature has shown dry particle shape depend on the dehydration condition and crystallization process. Hygroscopic tandem differential mobility analyzers (HT-DMA) are generally used to study the hygroscopic behavior of aerosol particles, however, it cannot provide the information about particle morphology and density. Therefore, in this study, in addition to a HT-DMA system, a hygroscopic coupled tandem DMA and aerosol particle mass analyzer (APM) were integrated and employed. The former size change and latter mass were used to derive the particle effective density and calculated dynamic shape factor which characterize particle shape.

The experimental results indicated that the solvent evaporation and solute diffusion dominated the morphology of the dry particles in dehydration process. In an extreme dry condition, the particle tended to form in irregular shape due to the fast remove of solvent. In contrast, there was more sufficient time for the solute diffusion in slow drying and the particle formed in spherical shape. However, drying and crystallization of aqueous aerosol particle were complicated process. Numerous factors such as materials, solute concentration, and particle size could affect the dry particle morphology. Thus, in order to investigate the dehydration process of aerosol particle, this study combined the diffusion equation and Köhler theory. In addition, quantifying the competitive relationship between solvent evaporation and solute diffusion by the dimensionless parameter: Peclet number and revealing the mechanism of particle formation in different experimental parameters setup. To understand the ability of nanoparticles to activate as cloud condensation nuclei in different drying condition. This study also conducted the HT-DMA-CCNC measurement and showed the activated fraction could be influenced by particle morphology.

4AP.6

Impact of Turbulence Parameters Influences on New Particle Formation Events in August Beijing. HAO WU, Fang Zhang, Zhanqing Li, Peng Yan, Yuying Wang, Xiaoai Jin, Xinxin Fan, *Beijing Normal University*

The Turbulent Kinetic Energy (TKE) affects convection, turbulence and entrainment, which can thus alter nucleation process due to the turbulent mixing that influences local supersaturation of precursor gases during New Particle Formation (NPF). During our experiment conducted in Beijing in August, we noted that the KTE occurs half an hour earlier than the particle burst. A further investigation of these cases suggests that the surface turbulence has a close relationship with the NPF event. A possible explanation is that short-time local supersaturation can trigger the binary nucleation process. Furthermore, we compared the Bowen Ratio (BR) with the growth rate (GR) and the condensation sink(CS), found that they are positively related. The Monin-Obukhov length(L) has a large fluctuation before the nucleation burst. Based on these findings, we proposed a kinetic mechanism of formation from the perspective of thermodynamic, and further explore the TKE and BR together with L as an indicator of NPF, association with other parameters such as Photosynthetically Active Radiation (PAR) or Net Radiation (NR) simultaneously. As aerosols won't affect climate much until they grow to certain size, typically over tens of nm when they can be activated to form cloud droplets, Such particles are referred to as Cloud Condensation Nuclei.

4AP.7

Mathematical Modeling of Aerosol Formation from Binary Vapor Mixtures. Ali Rostami, Sergey Fisenko, SERGEY N. MAXIMOFF, David Kane, Yezdi Pithawalla, Mohamed El-Shall, *Altria Client Services LLC*

Characterizing the aerosol produced by an Electronic Nicotine Delivery System (ENDS) is necessary for regulatory compliance and for designing and optimizing device performance. ENDSs produce condensation aerosol by mixing a high temperature vapor mixture with ambient air, resulting in a vapor mixture at high supersaturation. To characterize the resulting aerosol, it is important to estimate the homogeneous condensation nucleation rate, droplet size distribution, droplet composition as well as vapor-liquid partitioning. In circumstances where the supersaturation is very high and the critical cluster size is smaller than a dimer, the Classical Nucleation Theory (CNT) does not apply.

We addressed this limitation by developing a computational model that uses kinetic theory of gases to calculate nucleation rate and aerosol formation for binary mixtures of propylene glycol (PG) and glycerin (G) vapors. The process involves ternary collision of two vapor molecules of different kinds and any third molecule. The model accounts for non-isothermal growth of clusters with free molecular regime approximation where the cluster size is much smaller than the mean free path of vapor molecules. The latent heat of phase change, that affects the temperature difference between clusters of molecules and gaseous mixture, was accounted for in the model. An ideal liquid mixture solution was assumed for the droplets to account for the vapor-liquid partitioning of each constituent. After 200 ns of free molecular condensation the main mechanism responsible for droplets growth will be coagulation.

Computations were performed for different PG/G mixture ratios, ranging from 0/100 to 100/0 (mole based). Under ideal adiabatic mixing with air, at a vapor temperature of 570 K (close to glycerin boiling temperature), the initial supersaturation of glycerin drops several orders of magnitude. Particle size distribution over time and particle composition were calculated and presented. It was shown that final droplet size distribution is determined by coagulation. The temperatures of droplets and gaseous mixture are the same, due to high heat transfer coefficient at the particle-gas interface. The droplet composition for PG/G mixture strongly depends on the glycerin partial supersaturation in the initial mixture. The mass median diameter of aerosol particles, 1 s after mixing reaches 1-1.5 µm, and shows small dependence on the PG/G ratio and temperature. For all practical purpose, coagulation stops when the number density of micron size droplets decreases to less than about 10^{14} droplets/m^3.

4AP.8

Estimation of Atmospheric Columnar Organic Matter (OM) Mass Concentration from Remote Sensing Measurements.

YING ZHANG, Zhengqiang Li, Yang Lv, Yisong Xie, *Institute of Remote Sensing and Digital Earth, CAS*

Aerosols have adverse effects on human health and air quality, changing Earth's energy balance and lead to climate change. The components of aerosol are important because of the different spectral characteristics. Based on the low hygroscopic and high scattering properties of organic matter (OM) in fine modal atmospheric aerosols, we develop an inversion algorithm using remote sensing to obtain aerosol components including black carbon (BC), organic matter (OM), ammonium nitrate-like (AN), dust-like (DU) components and aerosol water content (AW). In the algorithm, the microphysical characteristics (i.e. volume distribution and complex refractive index) of particulates are preliminarily separated to fine and coarse modes, and then aerosol components are retrieved using bimodal parameters. We execute the algorithm using remote sensing measurements of sun-sky radiometer at AERONET site (Beijing RADI) in a period from October of 2014 to January of 2015. The results show a reasonable distribution of aerosol components and a good fit for spectral feature calculations. The mean OM mass concentration in atmospheric column is account for 14.93% of the total and 56.34% of dry and fine-mode aerosol, being a fairly good correlation (R=0.56) with the in situ observations near the surface layer.

4AP.10

Organic Aerosol Evolution from Wood Combustion Chamber during the Dilution Process. QIJING BIAN, Ezra Levin, Taehyoung Lee, Jeffrey R. Pierce, Sonia Kreidenweis, *Colorado State University*

Previous laboratory and field measurements have documented an increasing oxygenated fraction of organics during aerosol aging and atmospheric oxidation of compounds released in biomass burning plumes. In the laboratory burn experiments carried out as part of the FLAME III study, we diluted smoke stepwise under conditions of minimal oxidation, and observed an increase in the fractional contributions of less oxygenated compounds (C_xH_yO) and a decrease in the fraction of more oxygenated compounds ($C_xH_yO_z$), leading to a slight increase in the O:C ratio in the aerosols as the smoke was diluted. The volatility distributions for C_xH_y, C_xH_yO and $C_xH_yO_z$ were derived from the dilution data, and showed $C_xH_yO_z$ released during biomass burning has similar volatility distribution with C_xH_y but higher volatility than C_xH_yO. In addition, we also found that f60 (the fractional contributions of mass fragments with m/z 60, $C_2H_4O_2^+$, one of the species in $C_xH_yO_z$ family and a marker for biomass burning) decreased, and f44 (the fractional contributions of mass fragments with m/z 44, attributed by both CO_2^+ and $C_2H_4O^+$, and usually a marker of oxidized species) increased, with dilution in some burns. Our studies suggest that apparent trends in f44, aerosol oxidation state and O:C ratio observed in field measurements may not be due solely to oxidation processes, but may also have contributions from physical dilution processes occurring in biomass burning plumes.

4AP.11

Time-dependent Robin Boundary Condition for Convective Diffusion Equations. Panagiotis Neofytou, Marika Pilou, Christos Housiadas, YANNIS DROSSINOS, *European Commission, Joint Research Centre*

Convective diffusion of nanoparticles in bounded flows is an important transport mechanism in many industrial processes. Particle deposition via convective diffusion is of importance to, among others, scrubbers and filters, and aerosol measurement systems. An essential element in the calculation of nanoparticle deposition is the choice of the wall boundary condition. Under steady-state conditions, the wall boundary condition is usually taken to be totally absorbing, namely the particle concentration vanishes at the wall.

Microscopic considerations based on a generalized Fokker-Planck equation for the motion of a particle in a fluid suggest that a properly defined wall boundary condition relates the particle concentration at the wall to its derivative (at the wall). This boundary condition is known as the Robin boundary condition or radiation boundary condition. The associated constants (in the absence of external forces) depend on the particle diffusion coefficient, the particle thermal velocity, and the probability of particle adhesion to the wall (the momentum accommodation coefficient or the sticking fraction). As such, for most aerosol applications at atmospheric pressures and for high particle sticking probabilities the calculated deposition profile or total deposited mass do not depend on whether the Robin or the absorbing boundary is used. In fact, under these conditions the Robin boundary condition reduces to the absorbing boundary condition (i.e., a Dirichlet boundary condition).

The Robin boundary condition is common in systems where a heterogeneous reaction occurs at the wall because it connects the diffusive flux towards the wall to the particle flux that adheres to the wall. The proportionality constant is related to the heterogeneous reaction rate at the wall. Such relevant cases are encountered in, for example, biomedical uses of inhaled particles designed for targeted drug delivery at specific sites of the respiratory system.
We extended the Robin boundary condition to transient situations. Under non steady-state conditions an additional, first order derivative term appears in the time-dependent boundary condition. We investigated the conditions under which this additional time-dependent term influences deposition patterns of nanoparticles in various flows of interest in aerosol and biomedical applications (e.g., in laminar pipe flow).

4AP.12

Comparison of the Particle Growth Rates at Three Background Stations in the Czech Republic. Adéla Holubová Šmejkalová, HELENA PLACHÁ, Bitter Miroslav, Nadežda Zíková, Vladimír Ždímal, *Charles University*

Atmospheric aerosols as ubiquitous particles affect besides human health also climate. One of the key phenomena strongly affecting climate is new particle formation (NPF) and their consequent growth. NPF has been observed in many types of environments and geographical locations (Dall'Osto et al., 2018, Kulmala et al. 2004, Pushpawela et al. 2018, Sitho et al. 2006).

NPF and growth rates are controlled by several factors (concentration of pre-existing aerosols, precursor gases, air masses origin, meteorological conditions, and solar radiation) that are closely related to a sampling site (Jeong et al. 2010 , Nieminen et al. 2012). To explore possible differences in particle growth rates at various locations, measurements of number size distributions of atmospheric aerosol at three background stations in the Czech Republic were carried.

Two stations - Ústí nad Labem (50°39´39"N, 14°2´35"E, 147 m a.s l.) and Lom (50°35´8"N, 13°40´ 24"E, 265 m a.s.l.) are situated in northern, industrial part of the Czech Republic. Ústí nad Labem is urban background station in residential and commercial zone. Lom is rural background station in industrial and natural zone. National atmospheric observatory Košetice (NAOK – 49°34´24"N, 15°4´49"E, 534 m a.s.l.) is located in Czech-Moravian Highland. NAOK is rural background station in agricultural and natural zone.

The number size distributions were measured by aerosol spectrometers SMPS (IfT Tropos) in size range 10 to 800 nm. SMPS data were evaluated from March 1 to August 31, 2017. The growth rate (GR) of the particles freshly formed during the NPF event days was estimated by time evolution of the geometric mean diameter (GMD) of particles smaller than 100 nm. NPF event days were determined by Dal Maso et al. (2005) classification. Condensation sink (CS) was calculated by integration over the aerosol particle size distribution according to Kulmala et al. (2005).

Based on the calculated GR10, CS values and NPF frequencies, the three locations were compared. Results from 24/7 air quality monitoring gives evidence that Ústí nad Labem and Lom are more polluted locations than NAOK. Average PM10 concentrations at Ústí nad Labem and Lom fluctuated around 20 µg•m-3, SO2 ranged from 4 to7 µg•m-3 and NO2 varied between 8 and 19 µg•m-3. Average concentrations at NAOK were 15 µg•m-3, 2 µg•m-3 and 6 µg•m-3, for PM10, SO2 and NO2, respectively.

We observed 52 NPF event days at Lom, 47 NPF event days at NAOK and 43 NPF event days at Ústí nad Labem. GR10 was similar at Ústí nad Labem and Lom stations (median slightly over 3 nm•h-1). At NAOK, median of GR10 was 2.6 nm•h1. On average, CS was higher by a factor of 1.3 at Ústí nad Labem and Lom stations compared to NAOK (median 0.007s-1). Similarities of GR10 and CS between Ústí nad Labem and Lom stations can be caused by a common source, chemical industry, besides other things. In cases when GR was higher than median, pollutant concentrations were slightly higher, especially SO2 concentrations at Lom station.

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4AP.13

Numerical Study of Nano-Aerosol Generation through Rayleigh Fission of a Charged Viscous Liquid Drop. NEHA GAWANDE, Mohit Singh, Y.S. Mayya, R.M. Thaokar, *Indian Institute of Technology Bombay*

Electro-hydro-dynamic atomization is increasingly used for the production of nanoparticle aerosols. In this technique, a conducting liquid issuing from a needle maintained at a high electric potential with respect to ground, develops a Taylor cone from which highly charged primary droplets are ejected. The charges and the sizes of these droplets, which are generally in the range of several micrometers, depend on the various electro-hydro-dynamic properties of the system. These droplets further disintegrate into smaller droplets by successive Rayleigh fission events. Although the droplets are initially in the sub-Rayleigh limit, they gradually shrink to the radius (a) corresponding to the Rayleigh limit ($a^3=Qc/(64\pi^2\epsilon_0\gamma)$ where, Qc = charge on the droplet, γ =surface tension, ϵ_0=permittivity of free-space) due to evaporation. Although the Rayleigh fission process has been observed experimentally (Duft et al., 2003), the characteristics of the jet formed are still unclear. An understanding of the instability and breakup of such charged droplets from theoretical perspectives is essential for the effective design of the electrohydrodynamic system for the aerosol generation.

Towards this, we model (Gawande et al., 2017) the Rayleigh fission process of a perfectly conducting charged drop of a viscous liquid using a numerical scheme based on boundary element methods. The governing equations involve Laplace equation for the electric potential and Stokes equation for flow field. It is found from the simulations that the drop progressively deforms into a conical shape with pointed ends just prior to break up. As the numerical approach fails to predict charge ejection due to the occurrence of a singularity at this point, the charge loss fraction is estimated by determining how much minimum charge must be removed if the drop is to relax back to a spherical shape. In this manner, the charge loss due to Rayleigh fission (the difference between the original charge and the minimum charge removed) is estimated to be about 39%, which falls within the range of experimental data lying between 20% and 50%. The results on scaling laws, timescales of the process, and the role of various stresses on the dynamics of the drop are also discussed.

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4AP.14

Diffraction, Shadows and Scattering in Electrodynamics: A New View. Matthew Berg, CHRISTOPHER SORENSEN, *Kansas State University*

Diffraction is the spreading of waves of any kind. The mechanism of diffraction, however, can be quite different for different types of waves.

We show that for electromagnetic waves such as light the diffracted wave of an object is the Ewald-Oseen extinction wave in the far field. The intensity distribution of this wave yields what is commonly called the diffraction pattern. This is the same Ewald-Oseen extinction wave that extinguished the incident wave in the object and thereafter continued to do so immediately behind the object to create a shadow. The object can be an isolated particle or a screen with a hole; in the former case the Ewald-Oseen extinction wave is radiated from the particle, in the latter case it is radiated from the screen. This point of view explains Babinet's principle. If the object is an isolated, non-absorbing particle, nearly half the scattering cross section is in the Ewald-Oseen extinction wave; if the particle has significant absorption, nearly all the scattering cross section is contained there.

Unlike other common waves, such as sound and water waves, electromagnetic waves do not require a material medium in which to propagate. Thus a material object cannot block electromagnetic waves. Hence, light shadows do not form by blocking the light; light does not bend around the edges of the blocking object.

4AP.15

Physical and Optical Properties of Aerosols over Indo-Gangetic Basin. ASHOK JANGID, Suresh Tiwari, Ranjit Kumar, *DEI, Dayalbagh, Agra*

Aerosols are ubiquitous in nature and play a very important role in radiative forcing, climate change, visibility impairment, reduction in rain intensity and health-related issues. Aerosols have the variable behaviour of absorption and scattering of radiation due to nature of chemical constituents. Hence, estimation of radiative forcing of aerosols is important for which study on physical and chemical properties of aerosols is necessary. A systematic and long-term study on the understanding of properties of aerosols and its radiative forcing has been carried out at Agra over the Indo-Gangetic basin. The measurements of the mass concentration of aerosol (PM10 and PM2.5), black carbon (BC) and Aerosol Optical Depth (AOD) and monitoring of meteorological conditions have been performed. The mean concentration of PM10 (185.8 µg m-3), PM2.5 (94.2 µg m-3), black carbon (8.3 µg m-3) and AOD (0.93) has been determined. The concentration of PM10 and PM2.5 is 2-3 times higher than the NAAQS standard and 7-8 times higher than WHO standard. The high load of aerosol may be due to excessive vehicular emissions and road paved dust. Agra is surrounded by Rajasthan and lots of sand particles released from the grinding of marbles and red stone might be contributing towards a high load of aerosols. Black carbon concentration during night time may be also attributed to the increase in biofuel/biomass burning, especially for cooking as well as for heating purposes. The presence of fine mode particle enhances the radiance scattering and therefore, the aerosol optical depth (AOD) values are high at the shorter wavelength. Aerosol optical depth has been shown relatively strong wavelength dependence of optical depth at shorter wavelengths that generally decreases towards longer wavelengths irrespective of the seasonal change.

4AP.17

Characteristics and Relative Humidity Dependence of the Condensational Growth of Secondary Organic Aerosol Particles in a Continuously Mixed Flow Reactor. YUEMEI HAN, Jinghao Zhai, Chlóe Vercruysse, Yiming Qin, Jianhuai Ye, Scot T. Martin, *Harvard University*

Condensation of low volatility and semivolatile organic gas-phase species is an important atmospheric process for nucleated particles growing up to large sizes that might act as cloud condensation nuclei to impact the climate. The formation and subsequent growth of atmospherically relevant aerosol particles have been investigated extensively using laboratory environmental chambers. However, most of the previous studies are performed under limited relative humidity (RH) or even dry conditions, differing from those in the ambient atmosphere over a range of RH values. The influence of RH on the condensational growth and evolution of secondary organic material (SOM) remains poorly understood. In the current study, SOM was generated from the dark ozonolysis of alpha-pinene in a continuously mixed flow reactor, the Harvard Environmental Chamber, from dry to high RH conditions. The condensational growth of particle population was characterized from their number-size distributions measured in real-time using a scanning mobility particle sizer. The chemical composition of SOM particle was measured continuously with aerosol mass spectrometry. A strong nucleation of SOM particles occurred immediately after turning on the ozone lamp, followed by a series of particle growth events throughout the entire experiments. The chemical composition and oxidation state of SOM particles changed slightly with variable RH, which is possibly due to the influence of RH on the gas-particle partitioning of condensable organic compounds. The condensational growth rate and the time scale of growth will be derived from the evolution of particle number-size distributions for the individual RH values. The potential dependence on RH will be parameterized and incorporated into an analytical equation to optimize the characterization of condensational growth of SOM particle. Results from this study would be helpful to understand the gaps in the condensational growth of aerosol particles in laboratory studies compared to those in the real atmosphere.

4AP.18

Influence of Design Parameters and Operating Conditions on the Aerosol Produced by a Laskin Nozzle. BENOIT SAGOT, Louise Chazalon, Lyes Ait Ali Yahia, *ESTACA*

Oil separators are used in the automotive industry for the separation of oil mist from blow-by gases in internal combustion engines. These so-called “blow-by gases” result from leakages between the combustion chamber and the crankcase. These gases flow through the crankcase, which contains lubricating oil and the resulting oil mist, has to be cleaned up, for pollution control, oil consumption reduction and also to avoid turbo charger oil coking. To compare oil mist separators performances in laboratory, it is necessary to reproduce the engine operating conditions such as temperature and flow rates but also in terms of oil droplets distribution, and we developed such a laboratory bench.

A new generation of SI engine is currently under development, and new trends in engine design are a reduction of the engine size, an increase of the engine temperature, and a reduction of the oil viscosity. The targets are reduction of friction, increase of the overall efficiency, together with a reduction of the pollutant emissions. However, we observed that these changes in the design produced a strong increase of the overall oil mass concentration of blowby gases, which has been multiplied by a factor over 10. At the same time, the mean mass diameter of the aerosol distribution has been strongly reduced. We attribute this modification of the aerosol distribution to the reduction of the oil viscosity, and to higher cylinder pressure. Classical separation systems used in SI engines are based on impactors or cyclones. But to maintain the separation efficiency for the submicronic fraction of oil mists, car manufacturer are now using new systems that include filtration media, with high collection efficiencies and low pressure drop. For filter manufacturers, there is a new challenge: they test these filters on laboratory benches, with gravimetric measurements based on Andersen cascade impactors, and the downstream measurement time is very long (hours), since classical Laskin generators are not capable of producing a high concentration of the submicronic fraction of the aerosol. Therefore, for the submicronic fraction, there is a high uncertainty on the collection efficiency, even for long measurement times that also impose a high stability of the aerosol generation.

The aim of this study is to investigate the capacity of the Laskin nozzle to generate highly loaded oil mist with a low mean mass diameter, with a distribution equivalent to what is currently measured in under development SI engines. The first point is to quantify the impact of operating conditions such as oil temperature and gas flow rate in the Laskin nozzle, on the produced aerosol, in a wider range than what can be achieved with commercial devices such as the Palas PLG 2010.

We observed that for a given Laskin nozzle, the oil temperature has a strong impact of the overall oil concentration, with a limited variation of the mean mass diameter. These results are correlated to the reduction of the oil viscosity. The oil temperature was varied in the range 100°C to 200°C, and we observed a thermal degradation of the oil (SAE 0W30) for temperature higher than 160°C.

The flow rate in the Laskin nozzle has a strong impact on both the overall oil concentration, and on the aerosol distribution. The increase of the flow rate first produces an increase of the overall oil concentration. Then, a dilution effect appears, and we observe a bell shape curve for this oil concentration. However, for the submicronic fraction of the aerosol which is our main concern, the amount of oil droplets produced keeps increasing, which produces a reduction of the mean mass diameter. The last point of this study concerns an investigation of the influence of the geometrical parameters of the nozzle on the produced aerosol: for a fixed gas flow, we tested five nozzles with diameters in the range 0,3 to 1 mm. Based on Andersen cascade impactor gravimetric testing, the influence of the gas nozzle diameter was characterized.

With this experimental study, we were able to produce an oil mist distribution close to what is measured on under development SI engines. We got a better understanding of the way a Laskin nozzle works, which will be helpful for further development of filtration systems.

4AP.19

Light Scattering Analysis of Irregularly Shaped Dust Particles: A Study Using 3-Dimensional Reconstructions from Focused Ion-Beam (FIB) Tomography and Q-Space Analysis. DIANA ORTIZ-MONTALVO, Joseph Conny, *National Institute of Standards and Technology*

We study the scattering properties of irregularly shaped ambient dust particles. The way in which they scatter and absorb light has implications for aerosol optical remote sensing and aerosol radiative forcing applications. However, understanding light scattering and absorption by non-spherical particles can be very challenging. We used focused ion-beam scanning electron microscopy and energy-dispersive x-ray spectroscopy (FIB-SEM-EDS) to reconstruct three-dimensional (3-D) configurations of dust particles collected from urban and Asian sources. The 3-D reconstructions were then used in a discrete dipole approximation method (DDA) to determine their scattering properties for a range of shapes, sizes, and refractive indices. Scattering properties where obtained using actual shapes of the particles, as well as, (theoretical) equivalently-sized geometrical shapes like spheres, cubes, and tetrahedrons. We use Q-space analysis to interpret the angular distribution of the scattered light obtained for each particle. Q-space analysis has been recently used to distinguish scattering by particles of different shapes, and it involves plotting the scattered intensity versus the scattering wave vector (q or qR) on a log-log scale, where $q = 2k\sin(\theta/2)$, $k = 2\pi/\lambda$, and R = particle effective radius. Results from a limited number of particles show that when Q-space analysis is applied to 3D models of irregularly shaped particles (from FIB tomography), common patterns appear that agree with previous Q-space studies done on ice crystals and other irregularly shaped particles. More specifically, we found similar Q-space regimes including a forward scattering regime of constant intensity when $qR < 1$, followed by the Guinier regime when $qR \approx 1$, which is then followed by a complex power law regime with a -3 slope regime, a transition regime, and then a -4 slope regime. Currently, Q-space comparisons between actual and geometric shapes are underway with the objective of determining which geometric shape best represents the angular distribution and magnitude of the scattered light. Current work also focuses on the effects of the imaginary part of the refractive index on the light scattering of our dust particles. Preliminary data show that agreement between models for the geometric shapes and the actual shapes of particles varies substantially with particle size. Better agreements were observed for smaller particle sizes. Overall, shape and size cause more variability in the data than differences in chemical composition.

4AP.20

Physical Characterization of Tire Wear Particles Generated by Tire Simulator According to the Tread Wear Rate of Tires. SEOKHWAN LEE, Gibaek Kim, *Korea Institute of Machinery and Materials*

Vehicles emit particulate matter (PM) through their exhaust and non-exhaust sources. Exhaust PM can be generated by incomplete fuel combustion and lubricant volatilization. Non-exhaust PM can be emitted through tire, brake, and road wear processes and re-suspension of road dust. Due to the increasingly stringent regulations of the vehicle exhaust emissions, the relative contribution of non-exhaust PM become more significant. Among the non-exhaust PM, tire wear particles (TWPs) having relatively high uncertainty in physical properties have been less studied.

In this study, the tire simulator was operated in a closed control chamber (L: 3.5 m x W: 2.4 m x H: 2.2 m) to enable the detection of TWPs, thus excluding contamination particles originated from the other sources. TWPs were introduced into the sampling ports connected with several measurement instruments. DustTrack DRX, aerodynamic particle sizer (APS), fast mobility particle sizer (FMPS) spectrometer, condensation particle counter (CPC), and optical particle counter (OPC) were used to measure the various physical properties of TWPs such as number concentrations, number size distributions, mass size distributions, and mass concentrations (PM2.5 and PM10). The results suggest that the physical properties of TWPs can be affected by the tread wear rate of tires.

4AP.21

Aerosol Self-Cleansing by Dry Deposition in the Amazon Dry Season. FLORIAN DITAS, Christopher Pöhlker, Henrique Barbosa, Joel Brito, Samara Carbone, Xuguang Chi, Bruna A. Holanda, Isabella Hrabe de Angelis, Tobias Könemann, Jing Ming, Mira L. Pöhlker, Maria Prass, Daniel Moran-Zuloaga, Marta Sá, Jorge Saturno, Hang Su, Jian Wang, David Walter, Stefan Wolff, Alessandro Araujo, Paulo Artaxo, Ulrich Pöschl, Meinrat O. Andreae, *Max Planck Institute for Chemistry*

The Amazon rainforest is one of the few continental places where the atmospheric composition is episodically close to a pristine state. Local, regional and global anthropogenic pollution transported into the Amazon basin is chemically transformed and effectively deposited by wet and dry deposition.

This work focuses on observations in the central Amazon region – at the *Amazon Tall Tower Observatory* (ATTO). The ATTO site is equipped to measure aerosol microphysical, optical, chemical and morphological properties at two different measurement towers, which allows observations inside (5 m), close to (60 m) and well above (325 m) the forest canopy.

Vertically resolved meteorology and aerosol properties suggest a stable stratification during night resulting in a pronounced layering of aerosol particles. Frequent advection of pollution plumes during night leads to a massive increase of the aerosol burden above the canopy which is easily able to double the total number concentration. After sunrise, convection enables mixing and lofted aerosol layers are mixed downwards. Consequently, the particle concentration increases sharply close to and below the canopy. As soon as a well-mixed boundary layer is developed, particle properties are similar at all three measurement heights. In the course of the day, the total particle concentration features a pronounced decay which is to a certain degree related to the forest‘s self-cleansing capacity.

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4AP.22

Aerosol Optical Property Measurements of European Background Aerosol under Clean and Polluted Conditions.

SEBASTIAN DÜSING, Birgit Wehner, Albert Ansmann, Holger Baars, Ralf Käthner, Nan Ma, Thomas Müller, Patric Seifert, Holger Siebert, Gerald Spindler, Alfred Wiedensohler, Nicolas Bukowiecki, Joel Corbin, Martin Gysel, *Leibniz-Institute for Tropospheric Research*

Observations of the vertical distribution of aerosol are quite important since they allow to describe the radiative transport in the atmosphere. For this, remote sensing and airborne in-situ measurements are potential approaches to study the vertical aerosol distribution. But, both approaches underlie limitations and assumptions. Inter-comparison studies are therefore needed to a) compare the results of these approaches and b) to improve remote sensing algorithms and provide recommendations for vertical in situ measurements. Two campaigns were conducted and the results of these unique data-set for European background aerosol will be presented in this contribution.

Both campaigns took place in the vicinity of the rural ACTRIS (Aerosol, Clouds, and Trace gases Research InfraStructure Network) super-site at Melpitz (51.5° N, 12.9° E and 90 m above sea level).

In the first campaign (June 2015) 11 flights were conducted with a helicopter-borne payload up to a height of 2.3 km. This payload determined a) the ambient RH, T and b) the aerosol particle number size distribution (PNSD) within a particle diameter-range from 8 nm to 2.8 µm. Each flight contained horizontal flight legs of at least 10 min to determine statistically significant mean PNSD measurements. Three different instruments recorded the aerosol optical properties: particle light absorption (σ_{abs}) was determined by a small sized Aethalometer (AE51) at 880 nm wavelength whereas the Single Channel Tri-Colour Absorption Photometer (STAP) measured σabs at 450, 525, and 624 nm, while scattering (σ_{sca}) and extinction coefficient (σ_{ext}) were recorded with the Cavity Attenuation Phase Shift monitor (CAPSssa) at 630 nm wavelength.

In the second campaign (February/ March 2017) a box deployed on a tethered balloon included instruments determining σabs during 5 launches (AE51, STAP). The PNSD has also been detected within an optical particle diameter-range of 300 nm to 10 µm. All in situ measurements were conducted under dry conditions below 40% RH.

In both campaigns, the in situ measurements were complemented by a continuously running ground-based 3+2 multiwavelength polarization Raman lidar system PollyXT measuring profiles of the aerosol particle light backscatter coefficient (σ_{bsc}). Also we derived profiles of σext. Furthermore, an almucantar sun-photometer was measuring the aerosol optical thickness at different wavelengths.

These measurements were completed by measurements of the chemical aerosol composition as well as by measurements of the aerosol optical properties on ground. On the basis of the chemical composition measurements we derived the complex refractive index and the hygroscopicity of the aerosol particles.

Assuming that the chemical composition on ground is applicable for higher atmospheric altitudes, we first converted the in situ measured PNSD to its ambient state PNSD which has been used furthermore to calculate ambient state aerosol optical properties with a Mie theory based model.

Our measurements show that ground-based measurements are representative for the well-mixed planetary boundary layer. Furthermore, the in situ dry state modelled σ_{sca} and σ_{ext} showed good agreements with the airborne in situ measured equivalents. But especially the comparisons with filter-based absorption (σ_{abs}) instruments (STAP, AE51) and our Mie-calculations showed deviations which requires further research. Comparing the ambient state optical properties (model and in situ) with the measurements of the lidar, we detected cases were the model is in agreement (within measurement uncertainties) with the lidar observations. But we also observed also cases were the model calculated significantly lower σ_{ext} and values than observed by the lidar.

Not all flights/lunches are investigated yet, but conclusions and findings of the observations will be presented in this conference contribution.

4AP.24

Charge Size Distribution of Aerosol Nanoparticles Generated by Electrical Heating: Measurements and Theory.

MARIAM , Manish Joshi, Arshad Khan, B.K. Sapra, *Bhabha Atomic Research Centre, Mumbai*

Aerosol particles (natural and/or anthropogenic) are electrically charged, either because of the underlying formation mechanism or by their interactions with surrounding ionic environment. Knowledge of electrical behaviour of charged particles is applicable in several fields like drug delivery, electrostatic precipitators, residence time of aerosols etc. (Kwok et al., 2006; Pettersson et al., 2010). Type of aerosol particles as well as their generation method have a significant effect on the magnitude of the particle charge. This work focuses on estimation of charge size distribution (measurements and theoretical interpretation) of aerosols generated by electrical heating of nichrome wire using ELPI (Electrical Low Pressure Impactor). A laboratory made hot wire generator was used for generation of nanoparticle aerosols for this context (Khan et al. 2014). For steady conditions, charge per particle was found to be increasing from 0.009 to 1.305 for the size range of 9 to 230 nm (integral number concentration > 10^7 per cm^3). Depending on temperature, thermionic emission and surface ionization are responsible mechanisms, which operate when a metal is electrically heated. For the temperature under glowing conditions, surface ionization is dominant phenomenon and thermionic emission (threshold at much high temperature) is improbable. Theoretical comparisons of current density and polarity at varying temperature were made with experimental findings.

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4AP.25

Optical Properties and Chemical Constituents of Ambient Fine Particles in an Urban Environment of Korea. JONGBAE HEO, Seungpyo Cheong, Hwajin Kim, *Seoul National University*

Aerosol optical properties, chemical constituents, and sources of ambient fine particles were measured in Seoul, Korea, from May to November 2016. Light scattering (σscat) and absorption (σabs) coefficients were measured with a photoacustic extinctiometer (PAX) and a multiangle absorption photometer (MAAP), respectively. Chemical components of ambient fine particles were observed using a HR-ToF-AMS and their sources were identified using a positive matrix factorization model. During the study period, average mass concentration of fine particles, organic matter (OM), black carbon (BC), SO42-, NO3-, NH4+, and Cl- were 27.4 (±16.9) µg m-3, 13.0 (±8.3) µg m-3, 1.7 (±1.0) µg m-3, 5.0 (±3.6) µg m-3, 4.7 (±4.9) µg m-3, 2.9 (±2.3) µg m-3, and 0.3 (±0.5) µg m-3, respectively, and OM was a major component of fine particles. The observed σscat and σabs were 131.0 (±94.0) M m-1 and 13.6 (±8.2) M m-1, respectively. Both of the scattering and absorption coefficients showed unique diunal patterns with high peaks during the morning and evening rush hours due to the peak emissions of vehicles and the unfavorable meteorological conditions for dispersion of the vehicle emissions. The average of single scattering albedo calculated was 0.9 (±0.1), representing that fine particles in the study area contain relatively high fraction of scattering chemical components. The average mass scattering efficiency of fine particles was 4.70 m2 g-1 and exhibited higher values in spring and lower values in fall, showing a similar trend to mass of fine particles. This seasonal trend is influenced by the variations on chemical constituents of fine particles. Multiple linear regressions were performed to investigate associations of chemical components of fine particles with extinction coefficient (bext). Results showed that OM contributed the most to bext, accounting for 51.3%, followed by (NH4)2SO4, NH4NO3, and BC, 20.4%, 17.7%, and 9.7%, respectively. The PMF model identified four factors contributing to the OM, including low-volatile oxidized organic aerosol (LV-OOA), semi-volatile oxidized organic aerosol (SV-OOA), cooking influced organic aerosol (COA), and hydrocarbon like organic aerosol (HOA). Among the identified four factors, secondary organic aerosol factors (i.e. LV-OOA, SV-OOA) were the dominant contributors to bext. Therefore, reducing emissions of gaseous precursors corresponding to secondary aerosol formation may be important to improve both of air quality and visibility in Seoul.

4AP.26

Coagulation of Polydisperse Primary Particles from Free Molecular to Transition Regime. Georgios Kelesidis, EIRINI GOUDELI, *ETH Zürich*

Agglomeration of nanoparticles is encountered in both atmospheric and industrial processes as in volcanic plumes and aerosol manufacture of carbon black or fumed silica. Coagulation of polydisperse primary particles (PPs) in the transition regime is the dominant agglomerate growth mechanism in the low-temperature region of flame reactors and high-pressure environments of combustion engines. Even though the dynamics of coagulating spherical particles, such as self-preserving size distribution (SPSD) and coagulation rate are reasonably well-understood, there is significant uncertainty for fractal-like agglomerates. For the latter, coagulation rates have been proposed, their mobility and SPSDs have been determined. All these have been confined to agglomerates with monodisperse primary particles (PPs). Realistic agglomerates, however, consist of polydisperse PPs.

Here coagulation of nanoparticles of varying PP polydispersity (σg,PP = 1 – 3) in the absence of coalescence, sintering or surface growth is investigated by a discrete element method (DEM) (Goudeli et al., 2015) from the free molecular (Goudeli et al., 2016) to transition regime. The effect of PP polydispersity on agglomerate size (radius of gyration, mobility radius and volume-equivalent radius), morphology (fractal dimension, Df, mass mobility exponent, Dfm, and their prefactors) as well as on the attainment of the well-known asymptotic fractal-like structure (Df = 1.91 and Dfm= 2.15) and SPSD is investigated. Increasing the polydispersity of the constituent PPs from σg,PP = 1 to 3 does not affect but only delays the attainment of the asymptotic Df, Dfm and SPSD of the resulting agglomerates. Furthermore, the effect of PP polydispersity on agglomerate dynamics (coagulation rate and polydispersity) is elucidated quantitatively.

Such characteristics affect the environmental impact of agglomerates (climate forcing or visibility impairment by soot) or performance of gas sensors and catalysts.

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4AP.27

Single Scattering Albedo of Homogeneous, Spherical Particles in the Transition Region. HANS MOOSMULLER, Christopher Sorensen, *Desert Research Institute*

The aerosol single scattering albedo (SSA) is the dominant intensive particle parameter determining the aerosols radiative forcing in the earth's atmosphere [1-3]. We use Mie theory to examine the behavior of SSA as a function of size parameter x and complex refractive index m for homogeneous spherical particles. Previously, we investigated the limiting cases of the small particle limit ($x << 1$) and the large particle limit ($x >> 1$), where SSA is proportional to x^3 and independent of the size parameter x, respectively [4]. In between these cases lies the transition (or peak) region, where SSA transitions from the small to the large particle regime and, for sufficiently small imaginary parts of the refractive index, shows one or more peaks.

Here, we investigate the behavior of SSA in the transition region including conditions on the complex refractive index for peak formation, peak location, and general properties of SSA as function of size parameter.

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4AP.28

Fine Particle Formation in Corona Discharge. VALERY ZAGAYNOV, *National Research Nuclear University MEPhI*

The corona discharge is a gas discharge where geometry confines the gas ionizing process to high field ionization region around active electrode. The corona discharge can be used as a source of positive or negative charges based on the polarity of active electrode (Goldman et.al., 1985). It ought to be taken into account that some plasma is formed across the ionizing region causing ions and electrons colliding onto metal electrodes' surfaces. The energy of charged particles is sufficiently high capable of ionizing the gas molecules resulting from collision. Their energy could be at the level of tens of electron-volts corresponding to tens thousands degrees. It could be supposed that these impacts of electrons onto surfaces could cause some electrode erosion resulting from charged particles and electrons knocking atoms and molecules out of electrode's surface. Then, these displaced atoms and molecules turn into vapor molecules and contribute to the surrounding gas phase. Upon moving away from the ionizing region, the temperature of such vapor molecules rapidly decreases and, any unavoidable collision between each other could potentially move them to the bond states, subject to their ability to release excessive kinetic energy. Thus, fine particles composed of electrode material could be formed (Smirnov, 1999). To investigate this process the experimental set up has been constructed. The set up consists of silver particle generator and diffusion aerosol spectrometer (DAS) capable of measuring concentration and size distribution of produced silver particles. The particle generator consisted of thin silver needle (active electrode) and ring silver electrode. Particles produced in the active electrode region were measured by the DAS at one minute interval providing information about particle size distribution and concentration. Typical size distribution of silver particles produced by the above generator is shown in Figure 1. As is seen from this graph some part of generated particles is not presented in the figure, as it is laying beyond the bottom detection limit of DAS, which is blind for particles smaller than 3 nm. Analyzing the obtained experimental data enabled to estimate an amount of silver atoms (which took part in particle formation) generated by one electron impacting onto the active electrode surface (generation efficiency). To achieve this goal, the electric current of corona discharge, total particle concentration and particle size distribution were accurately measured and the results were used in calculations. Dividing measured electric current by electron charge the electron flow on electrode surface was calculated. Then number of silver atoms which took part in particle formation was estimated by measured particle size distribution and its concentration. On the ground of these estimations it was obtained that efficiency of particle generation is between 10-3 – 10-2. At the same time it has to be taken into account that this is low boundary estimation, because part of particles (most fine) was not recorded due to their location beyond the DAS detection limit. Size distribution of the particles, formatted in corona discharge.

The proposed approach to model nanoparticle generation in corona discharge by the vapor of silver or other metals is supposed to consider coagulation equation for corresponding conditions. This method is promoted by the fact that the vapor transition from hot ionizing region to the region with room conditions is very abrupt, and any collisions between particles could result in bond state. At the same time, this method of particle generation can be useful if very fine particles with narrow size distribution are required.

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Keywords: corona discharge, nanoparticles, particle formation

4AP.29

Temporal Variation of Particles Suspended (TSP, PM10 and PM2.5) and Composition Chemistry of PM10 in San Francisco de Campeche, México. ALBERTO ANTONIO ESPINOSA GUZMÁN, Javier Reyes Trujeque, Javier Miranda, Juan Carlos Pineda SantaMaría, Ana Luisa Alarcón Jímenez, María del Carmen Torres Barrera, Rodolfo Sosa Echevería, *Autonomus University of Campeche*

Air pollution is a global problem that affects both natural environment and human health. Currently, this issue is specially studied due to the higher demand on cleaner environment with low air pollution levels at urban areas, where a better life quality is desirable. In Mexico, studies on atmospheric particles and their effects on air quality and environmental impact, are widely developed in densely populated urban sites. That is the case of metropolitan areas such as Mexico City, Guadalajara, and Monterrey. Moreover, in Mexico smaller cities, such as San Francisco de Campeche (SFC), there is lack of air quality studies, including those related with atmospheric particles. SFC is located on the West coast of the Yucatan Peninsula in the state of Campeche, México.

SFC is bordering by the Gulf of Mexico. It is in the middle of a small valley, limited N, E by small hills. At the W, the Bay of Campeche delimits its coastal area. Some of those hills are subjected to continuous erosion episodes, building of residential developments, or are used to extract materials for construction. These very aggressive activities affect the land, causing dust storms, especially during the dry season. The last one increases local levels of atmospheric particles. During the spring, the City is regularly affected by the traditional farmlands burning produced at the region in order to prepare crops. Also, there appear numerous natural forest fires during dry periods, something that potentially could increase the content of pollutants in the atmosphere. In the last decade SFC increased its population by 17.3% (nowadays around 280,000 inhabitants). Also, the increase in the number of cars rinse the City with one of the most higher number of vehicles per capita in the country. The devices was installed on the roof of the “SEMARNTACAM”, it is located (19.82 N, -90.53 W), at the historic center of the city. The area is characterized by an intense economical and official activities. In this area, important traffic jams can be observed in streets surrounding the buildings along the day.

Elemental analysis for three fractions (TSP, PM_{10} and $PM_{2.5}$) was determined by using X-Ray Fluorescence (XRF). Samples were collected on 8 "x10" quartz fiber filters (Whatman). High volume samplers (Tisch Environment) were used, according to the Official Mexican Standard NOM-035-SEMARNAT-1993. An ion analysis was also carried out for the PM_{10} fraction, using the Ion Chromatography (IC) technique. The sampling period was from November 1st 2014 to October 30th 2015, each three days during 24 hour. Sampling initiated at 8:00 am.

XRF indicated the presence of Al, Si, P, S, Cl, K, Ca, Ti, Cr, Mn, Fe, Cu, Zn and Sr predominant elements. Cluster analysis (AC) determined associations between: K and S; due to smoke emissions probably from the burning of crop fields; Cr, Mn, Cu, (industrial emissions); Ca, Ti and Fe (raising dust). Ionic analysis determined the species: Na^+, K^+, Mg^{2+}, Ca^+ 2, Cl^-, NO^{-3}, $SO4^{-2}$, $HCO3^-$ and high concentrations were of $SO4^{-2}$, Cl^- , Na^+, in dry season for this study. Principal Component Analysis (PCA) applied to ion concentration in PM10 indicating that the contribution the Na^+, Cl^- and Mg^{2+} is due for marine aerosol, Ca^{2+} due crustal origin and NO^-_3, SO_4^{-2} suggests vehicular emissions. Also back-trajectories models showed that biomass burning at farming areas affects the concentration of TSP and PM10 during the dry season.

4CA.1

Sources of PM2.5 Carbonaceous Aerosol in Riyadh, Saudi Arabia. QIJING BIAN, Badr Alharbi, Mohammed M. Shareef, Tahir Husain, Mohammad J. Pasha, Samuel Atwood, Sonia Kreidenweis, *Colorado State University*

Knowledge of the sources of carbonaceous aerosol affecting air quality in Riyadh, Saudi Arabia is limited, but needed for the development of pollution control strategies. We conducted sampling of PM2.5 from April to September, 2012 at various sites in the city, and used a thermo-optical semi-continuous method to quantify the organic carbon (OC) and elemental carbon (EC) concentrations. The average OC and EC concentrations were 4.7 ± 4.4 and 2.1 ± 2.5 µg m-3, respectively, during this period. Both OC and EC concentrations had strong diurnal variations, with peaks at 6-8 am and 20-22 pm, attributed to the combined effect of increased vehicle emissions during rush hour and the shallow boundary layer in the early morning and at night. This finding suggested a significant influence of local vehicular emissions on OC and EC. The OC/EC ratio in primary emissions was estimated to be 1.01, close to documented values for diesel emissions. Estimated primary (POC) and secondary (SOC) organic carbon concentrations were comparable, with average concentrations of 2.0 ± 2.4 and 2.8 ± 3.4 µg m-3, respectively.

We also collected 24 hour samples of PM10 onto quartz microfiber filters and analyzed these for an array of metals by ICP-OES. Total OC was correlated with Ca (R2 of 0.63), suggesting that OC precursors and Ca may have similar sources, and the possibility that they underwent similar atmospheric processing. In addition to a ubiquitous dust source, Ca is emitted during desalting processes in the numerous refineries in the region and from cement kilns, suggesting these sources may also contribute to observed OC concentrations in Riyadh. Concentration weighted trajectory (CWT) analysis showed that high OC and EC concentrations were associated with air masses arriving from the Persian Gulf and the region around Baghdad, locations with high densities of oil fields and refineries as well as a large Saudi Arabian cement plant. We further applied positive matrix factorization to the aligned data set of EC, OC and metal concentrations (Al, Ca, Cu, Fe, K, Mg, Mn, Na, Ni, Pb and V). Three factors were derived, and were proposed to be associated with oil combustion, industrial emissions (Pb-based), and a combined source from oil fields, cement production, and local vehicular emissions. The dominant OC and EC source was the combined source, contributing 3.9 µg m-3 (80%) to observed OC and 1.9 µg m-3 (92%) to observed EC.

4CA.2

Hydroxyl and Nitrate Radical Aging of Organic Emissions from Wildfires. SHANTANU JATHAR, Ali Akherati, Shiva Tarun, Liam Lewane, Abril Galang, Timothy Onasch, Scott Herndon, Joseph Roscioli, Tara Yacovitch, Edward Fortner, Philip Croteau, Wen Xu, Conner Daube, Berk Knighton, Benjamin Werden, Ezra Wood, Christopher Lim, David Hagan, Christopher Cappa, Jesse Kroll, Daniel S. Tkacik, Christopher Hennigan, Allen Robinson, *Colorado State University*

Wildfires are the largest combustion-related source of organic emissions to the atmosphere; these include direct emissions of primary organic aerosol (POA) and semi-volatile, intermediate-volatility, and volatile organic compounds (SVOCs, IVOCs, and VOCs). However, there are large uncertainties surrounding the evolution of these organic emissions as they are physically and chemically transformed in the atmosphere. To understand these transformations, we performed sixteen experiments using an environmental chamber to simulate day- and night-time chemistry of wildfire emissions from 6 different fuels at the Fire Laboratory in Missoula, MT.

Across the test matrix, the experiments simulated 0.5 to 9 hours of equivalent day-time aging (with the hydroxyl radical and ozone) or several hours of night-time aging (with the nitrate radical). Day-time aging resulted in an average organic aerosol (OA) mass enhancement of 72% although the full range of OA mass enhancements varied between ~0% and 400%. The distribution of OA mass enhancements was consistent with chamber and flow reactor experiments performed at the Fire Laboratory in 2010 and 2012 but similar to previous studies offered no evidence to link the OA mass enhancement to fuel type, burn conditions, or oxidant exposure. The chamber OA mass enhancements were nearly half of those observed with flow reactor experiments performed in conjunction with this study and the differences could be explained by significant differences in oxidant exposure (median age of 6.1 hours for the chamber versus 3.8 days for the flow reactor). Night-time aging resulted in an average OA mass enhancement of 20%, which was lower than that observed with day-time aging. We found strong evidence for production of organic nitrates during the night-time experiments where they accounted for ~10% of the total OA emitted and formed by the end of the experiment. Both day- and night-time aging resulted in only modest changes in the OA composition measured by the aerosol mass spectrometer. The median fraction of the OA mass measured at a mass-to-charge ratio of 44 and 60 changed by +65% and -25% respectively and the median oxygen-to-carbon ratio increased by 25%. The flow reactor experiments witnessed much larger changes in the OA composition (e.g., median oxygen-to-carbon ratio more than doubled), which again could be attributed to substantial differences in oxidant exposure.

Ongoing work is focussed on integrating chamber and flow reactor wildfire experiments from 2010, 2012, and 2016 (~130 individual experiments) to examine the relationship between OA mass enhancement ratios, modified combustion efficiency, initial aerosol concentrations and composition, aerosol size, oxidant exposure, VOC:NOx ratios, and emissions and speciation of SOA precursors.

4CA.3

Trend of Elemental and Organic Carbon (EC/OC) Concentrations at the National Atmospheric Observatory Košetice (Czech Republic) in 2009-2016. MILAN VANA, Adéla Holubová Šmejkalová, *Czech Hydrometeorological Institute*

Carbonaceous aerosol particles in the atmosphere are formed mainly of elemental carbon and organic compounds (Seinfeld, Pandis 2006). Elemental (EC) and organic carbon (OC) are the products of imperfect combustion of organic materials (coal, oil, petrol, wood and biomass); sources of OC also include the resuspension of dust, which is related to transport, and biogenic particles. While EC is emitted into the atmosphere only directly, OC can be formed by the reactions of gaseous organic precursors. The large number of toxicological studies collected in the WHO document of 2012 are related to the negative effects of carbonaceous aerosols on human health. Regular EC/OC measurement has been implementing at the National Atmospheric Observatory Košetice (NAOK) since 2009 within the framework of EU-projects EUSAAR (European Supersites for Atmospheric Aerosol Research) and later ACTRIS (Aerosols, Clouds, and Trace gases Research Infrastructure Network) and ACTRIS-2. Sampling frequency is every 6th day on 2 quartz-fibre filters. The samples are analyzed using EC-OC Sunset Lab Dual Analyzer. In 2013, a parallel measurement using a field semi-online OC/EC analyzer from Sunset Instrument started. Both instruments sampled an aerosol fraction PM2.5 and denuders were used to remove volatile organic compounds. Automatic optical corrections (based on a laser transmission monitoring) for charring were made during each thermal-optical analysis. The presented trend study is based on manual data, the data from the analyzer were used only for completing the data series when the manual data is missing. Kosetice Observatory, operated by the Czech Hydrometeorological Institute (CHMI), was established in 1988. The observatory is located in free area outside of settlement (49°35´ N, 15°05´E, 534 m above sea level) and represents the Czech Republic in several international long-term monitoring programmes (EMEP, GAW). Detailed information is available at (Vana et al., 2013).The used statistical method for trend analysis in this study is based on the nonparametric Mann-Kendall test for trend and the nonparametric Sen's method for the magnitude of the trend. The EC emissions in the Czech Republic display continuously decreasing trend from 4,8 (kt) in 2009 to 3,2 kt in 2015. This tendency is reflected in the statistically significant downward trend of EC concentrations at NAOK from 0,6 µg.m-3 in 2009 to 0,3 µg.m-3 in 2016. Slightly decreasing trend was found both in cold (October-March) and warm (April-September) period. The difference between the seasons in not visible. OC concentrations shows decreasing tendency, which is not statistically significant. In the period 2009-2013 the mean annual concentrations stagnated round 3,5 µg.m-3 and then dropped under 3 µg.m-3. The similar tendency is visible also in the cold period. On the other hand, in the warm period, no trend was found. The mean annual ratio of EC on total carbon (TC) was 13%. No visible tendency was found during the period under review. In the warm period, the ratio was lower (11%) with decreasing tendency. On contrary, significant upward trend of the ratio was found in the cold period (mean annual ratio 15%).

The research leading to these results has received funding from the project for support of national research infrastructure ACTRIS – participation of the Czech Republic (ACTRIS-CZ - LM2015037) – Ministry of Education, Youth and Sports of the Czech Republic.

4CA.4

Roadside Measurements of Black Carbon, PM2.5, Particle Number and NOx Vehicle Emission Factors in Brazil.

PATRICIA KRECL, Admir Créso Targino, Thiago Landi, Matthias Ketzel, *Federal University of Technology*

The road transportation sector contributes largely to air pollution in urban areas, and accurate knowledge of vehicle emission factors (EF) is crucial to prepare reliable emission inventories which, in turn, are strategic tools for air quality management. Curbside and rooftop concentrations of several traffic-related species were measured within a busy street canyon in Londrina (Brazil) and EF for NOx, black carbon (BC), fine particles ($PM_{2.5}$) and particle number (N) were calculated based on these measurements and inverse modeling using the Operational Street Pollution Model (OSPM). We highlight the importance of this work in quantifying the effects of possible off-cycle BC, $PM_{2.5}$, NOx and N emissions in urban areas by measuring emissions in real driving conditions in a continent-sized country where there is a lack of EF studies. On average, one heavy-duty vehicle (HDV) emitted more pollutants than one light-duty vehicle (LDV) with EF_{HDV}/EF_{LDV} ratios of 27, 12, 10 and 4 for BC, NOx, $PM_{2.5}$ and N, respectively. Our results are consistent with literature values reported by other studies conducted also under real-world driving conditions in Brazil (São Paulo city). As far as we know, we report the first EFN ever measured in Brazil and when compared to other works carried out in street canyons in Europe, they were similar for the HDV fleet but much higher for the LDV fleet. Our EF are much higher than laboratory measurements conducted in Brazil and Europe, especially for particles. This finding suggests that the EF derived from laboratory tests should be revised for all vehicle categories in Brazil, since they are used to compile official national inventories for the road transportation sector and also to assess their associated health and climate (in the case of BC) impacts. Finally, Brazilian regulators should incorporate certification procedures that more closely resemble real-world conditions. For example, adopting certification tests in laboratory that consider cold-start and low-speed driving and also real drive emission (RDE) testing already in place in the European Union. There is also a need of quantifying the non-exhaust EF for particulate matter and determine mileage deterioration for all pollutants and vehicle categories, which are missing in all official inventory calculations.

4CA.5

Sources of Brown Carbon in Urban Environments: Importance of Vehicular Emissions. NETHMI KASTHURIARACHCHI, Max Adam, Yue Liang, Dong Zhang, Alex Lee, *National University of Singapore*

Carbonaceous aerosols are known to affect the global climate through direct absorption and scattering of solar radiation. While black carbon (BC) is the most efficient light absorbing aerosol, brown carbon (BrC) has been found to efficiently absorb radiation in the near UV and visible wavelengths. Although biomass burning has been extensively studied as a primary source of BrC, there is increasing laboratory evidence that incomplete fossil fuel combustion, such as vehicular emissions, can be a potential source of BrC in urban environments with minimal influence from biomass burning.

In this study, a seven-wavelength Aethalometer (AE33, Magee Scientific), which gives loading factor-corrected absorbance measurements at 370nm, 440nm, 520nm, 590nm, 660nm, 880nm and 950nm, was deployed to measure ambient BC and BrC in Singapore. A co-located soot-particle aerosol mass spectrometer (SP-AMS, Aerodyne Research) was used to measure non-refractory chemical composition of ambient particles. No biomass burning episodes due to transboundary smoke were reported during the month-long sampling period. The mean absorption Ångström exponent (AE) of ambient particles was 1.06 ± 0.05, further indicating the absence of biomass burning influence (i.e., AAE > 2 for biomass burning smoke). Comparison of ambient and thermodenuded (at 200^{o}C) particles confirms the presence of BrC in ambient particles. Assuming AAE of ambient pure BC is equal to 1, the light absorption properties of ambient BrC were quantified. The mean AAE of BrC was estimated to be in the range of 3 to 4, which is comparable to the values measured in urban environments with strong influence from fossil fuel combustion.

Positive matrix factorization (PMF) of organic fragments measured by SP-AMS identified four major types of organic aerosols, including hydrocarbon-like organic aerosols (HOA), cooking-related organic aerosols (COA) and less and more oxidised oxygenated organic aerosols (LO-OOA and MO-OOA). Out of the four types of organic aerosols, HOA showed the strongest correlation ($r^2 = 0.6$-0.7) with the BrC absorbance at 370nm. HOA are known to be emitted from vehicles and off-road engines and showed strong correlation with BC absorbance at 880nm ($r^2 > 0.75$). For the total absorption at 370nm, multiple linear regression analysis for BC and the four organic aerosol components gave the mass absorption coefficient of HOA ($MAC_{HOA,370nm}$, m^2/g), a measurement proxy of BrC, approximately equal to 1.22 m^2/g. This value is comparable to the reported MAC_{365nm} values of biomass burning organic aerosols. Multiplying the MAC for each component by the mean mass concentration showed that HOA contributed up to ~6% and ~70% of total (i.e., BrC + BC) and BrC absorbance at 370 nm, respectively. Overall, our preliminary results provide field evidence to highlight that vehicular emissions can be an important source of ambient BrC in urban environments. Volatility of ambient BrC and organic aerosols based on the thermodenuder measurements will be discussed.

4CA.6

Over a Decade-long Trend of Concentrations of Ultrafine Particle and Carbonaceous Aerosols at a Traffic Intersection.

YUJI FUJITANI, Katsuyuki Takahashi, Akihiro Fushimi, Shuichi Hasegawa, Yoshinori Kondo, Kiyoshi Tanabe, Shinji Kobayashi, *National Institute for Environmental Studies*

This study showed long-term monitoring data (2004-2017) of particle number concentrations (PNCs: particle size 10-480 nm), size-resolved particulate matter (PM) mass and carbon component, and atmospheric pollutants at the traffic intersection in a metropolitan area in Japan. Comparison was made between atmospheric concentrations of these pollutants at the traffic intersection and the tailpipe PM mass emissions from diesel trucks that passing through the traffic intersection, which is estimated from traffic volumes as a function of emission regulation year and gross weight of trucks obtained by license plate numbers research and giving emission factor of each category.

Decay rate of concentrations of elemental carbon in $PM_{0.1}$ and in $PM_{2.5}$ from 2005 to 2016 were excellently match with reduction rate of PM tailpipe emissions, which indicates tailpipe emission of diesel trucks was dominant source of atmospheric PM and the reduction in atmospheric concentrations directly reflected cleaner of traffic exhausts. From the traffic information, not only reduction of traffic volume during the period but also replacing vehicles that comply with tighter regulation were forward to reduce emissions, which also resulted in better correlations between atmospheric concentrations and tailpipe PM mass emission rather than traffic volume. On the other hand, slower decrease trend of exhaust related PNC than decrease trend of tailpipe PM mass emissions were found.

The positive matrix factorization (PMF) analysis using year-to-year data of PNCs and EC showed the largest contribution factor to EC in $PM_{2.5}$ (about 50% in entire period average) attributed to tailpipe emission from the trucks of emission regulation of 1997-99 because emissions of this regulation vehicles also contribute about 50% to total tailpipe PM mass emission. As for PN particle smaller than 100 nm in entire period of winter, factors that attributed to emissions from 1988-94 regulation vehicles contribute about 50%. The result of PMF analysis, diurnal trend of pollutants, and comparison between summer and winter seasons suggested that high PN in winter morning is due to nucleation of semi-volatile gases mainly emitted from 1988-94 regulation vehicles concurrently in a cold temperature, low wind speed, and low height mixing layer. The implement policy of emission regulation in terms of PM mass did not effective to reduce atmospheric PN as much as PM mass otherwise removing semi-volatile gases which are co-pollutants of PM.

4CA.8

Influence of Aerosol Sources on Atmospheric Black Carbon Absorption Enhancement in the Region of Paris, France.

YUNJIANG ZHANG, Olivier Favez, Francesco Canonaco, Dantong Liu, Jean-Eudes Petit, Tanguy Amodeo, Nicolas Bonnaire, Francois Truong, Jean Sciare, Andre S.H. Prévôt, Valerie Gros, Alexandre Albinet, *INERIS*

Atmospheric black carbon (BC) and light-absorbing organic aerosol (also referred as brown carbon, BrC) have strong effects on the Earth’s climate by absorbing direct solar radiation. To better characterize and quantify these effects, a better understanding of specific underlying mechanisms is needed such as the influence of primary emissions and secondary processes on absorption properties over long-term periods. We report here results of a three-year continuous field observations conducted from March 2014 to March 2017 at a suburban background station (SIRTA) in the Paris region (France). Submicron nonrefractory aerosol species were measured in near real-time using an aerodyne aerosol chemical speciation monitor and were apportioned using Positive Matrix Factorization (PMF) analysis to identify and quantified major organic aerosol (OA) sources. Light absorption properties of BC and BrC were determined by direct measurements using a 7-wavelength aethalometer equipped with the dual spot technology. Co-located 24-h filter-based analyses were performed by thermo-optical technique to quantify the mass concentration of elemental carbon (EC) in $PM_{2.5}$. Absorption enhancement (E_{abs}) of BC-containing particles was obtained using mass absorption coefficient (MAC) ratios calculated between observed (= babs / [EC]) and expected values for uncoated BC. Results showed that the observed Eabs significantly increased with the mass ratio of secondary aerosols to EC, suggesting a strong influence of this secondary components on BC absorption enhancement. Important BrC contribution to the total absorption in the near UV could be attributed to residential wood burning activities in winter and led to significant E_{abs}, independently of internal or external BrC mixing with BC particles. Finally, new findings on summertime aerosol optical properties are also presented and discussed here.

4CA.9

Gaseous and Speciated Particulate Emissions from the Open Burning of Wastes from Tree Pruning. CÉLIA ALVES, Ana Vicente, Estela Vicente, Margarita Evtyugina, María Fernández-Amado, Purificación López-Mahía, *University of Aveiro*

Open-air burning of wastes from tree pruning is a common practice in many regions worldwide. However, this practice degrades air quality and contributes to the greenhouse effect. Aiming at characterizing the gaseous emissions, the smoke from the open burning of vine, olive, willow and acacia branches was sampled into Tedlar bags. In parallel, a high volume sampler was used to collect PM_{10} on quartz filters. The gaseous compounds in Tedlar bags were assessed using a Fourier transform infrared gas analyzer. PM_{10} filters were subjected to the following determinations: ion chromatography, organic and elemental carbon (OC and EC) by a thermo-optical technique, and organic speciation by gas chromatography-mass spectrometry after multisolvent extraction. Emission factors were calculated by stoichiometric considerations using the carbon mass balance method and were as follows (g/kg biofuel, dry basis): 1564-1663 CO_2, 40.6-87.7 CO, 2.06-5.82 CH_4, 0.91-3.73 ethane, < 0.99 ethylene, < 1.80 formaldehyde, 2.70-7.44 OC, 0.32-1.18 EC, and 8.76-20.1 PM_{10}. The modified combustion efficiency (MCE) was always higher than 0.95, suggesting predominance of flaming combustions. MCE was strongly correlated with CO_2 and anticorrelated with CO. From the PM_{10} emitted, water soluble ions represented from 5.3 % (vines) to 12.7 % (acacia). Potassium was the dominant ionic species, accounting for a PM_{10} content from 1.4 to 4.7 % wt. While in smoke from vines and olive combustion the NaCl mass fractions were lower than 0.9 %, higher weight percentages were obtained for willow (3.6) and acacia (6.7). On average, OC accounted for PM_{10} mass fractions of 33.4, 19.3, 32.3 and 36.5 % for willow, acacia, vines and olive, respectively, whist EC represented 5.04, 2.34, 3.53 and 7.32 %, by the same order. Mean levoglucosan (L) mass fractions of 18.1, 13.2, 17.1 and 12.4 mg/g PM_{10} were obtained in samples from the combustion of vines, olive, willow and acacia, respectively. The ratios between this anhydrosugar and its stereoisomers, mannosan (M) and galactosan (G), were within the wide range of values reported for other sources, such as residential biomass burning of hardwood and softwood, forest fire smoke or grass combustion [1]. In the present study, the mean ratios varied from 4.2 and 8.8 for L/M and between 2.3 and 3.7 for L/(M+G). PAH emissions from the combustion of vines and olive branches were one order of magnitude higher than those from acacia and willow. PAHs with 3 or 4-rings were dominant. Among these, the most representative in terms of mass concentrations (µg/g PM_{10}) were: acenaphthylene (27.7-90.9), fluorene (92.7-133), phenanthrene (3.96-281), fluoranthene (17.8-510), pyrene (22.7-511), and chrysene (16.5-545). Benzo[a]pyrene is often used as a surrogate for all carcinogenic PAHs. Its mean mass fractions ranged from 6.51 (willow) to 91.3 (vines) µg/g PM_{10}. Retene, commonly pointed out as a molecular tracer of softwood combustion, was always present (8.23-18.9 µg/g PM_{10}), regardless of the pruning residue. The detection of this polyaromatic in particles from multiple sources raises doubts about its suitability as a tracer for the combustion of conifers [2]. The new databases of the present study can potentially contribute to more accurate source apportionment results when applying receptor models, as well as to improve emission inventories.

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[1] Fabbri et al. (2009) Atmos. Environ. 43, 2286.
[2] Vicente E.D., Alves C.A. (2018) Atmos. Res. 199, 159.

4CA.10

Sources and Physicochemical Characteristics of Black Carbon Aerosol in the Southeastern Tibetan Plateau: Internal Mixing Enhances Light Absorption. QIYUAN WANG, Junji Cao, Yongming Han, *Institute of Earth Environment, Chinese Academy of Sciences*

Black carbon (BC) aerosol over the Tibetan Plateau (TP) has important effects on regional climate and hydrological processes. An intensive measurement campaign was conducted at Lulang (~3300 m above sea level), southeastern TP, from September to October 2015 to investigate the sources and physicochemical characteristics of refractory BC (rBC) aerosol. The grand average rBC mass concentration was 0.31 ± 0.55 $\mu g\ m^{-3}$, which is higher than most BC results for the TP. A clear diurnal cycle in rBC showed high values in the morning and low values in the afternoon. A bivariate polar plot showed that rBC loadings were affected by wind speed and direction, which was used to infer the dominant transport directions. The estimated net surface transport intensity for rBC was +0.05 ± 0.29 $\mu g\ s^{-1}\ m^{-2}$, indicating that stronger transport from outside the TP compared with the interior of the TP. Cluster analysis and a concentration-weighted trajectory model indicated that emissions from north India had important contribution to the high rBC, but the effects of internal TP sources cannot be overlooked. The average mass median diameter (MMD) of rBC was 160 ± 23 nm, with smaller size on rainy days (145 nm) compared with non-rainy days (164 nm). The average number fraction of thickly-coated rBC (F_{rBC}) was 39 ± 8%. The FrBC increased with the enhanced O3 mixing ratio from 10:00–14:00 local time, indicating that the photochemical oxidation played an important role in forming rBC coatings. The average rBC absorption enhancement (E_{abs}) was estimated to be 1.8, suggesting that light absorption by coated rBC particles was greater than that for the uncoated ones. The Eabs was strongly positively correlated with the FrBC, indicating an amplification of light absorption for internally-mixed rBC. When rBC core 170 nm. Our study provides insight into the sources and evolution of rBC aerosol on the TP. It is useful for further modelling studies improving precise of evaluating the radiative forcing of carbonaceous aerosols in this area.

4CA.11

Characteristics of Pollutant Emissions from Typical Coastal and Riverine Ships in China. XIANG DING, Qing Li, Di Wu, Jianfeng Sun, Xianmang Xu, JianMin Chen, *Fudan University*

China accounted for 70% of the world's top 10 ports in 2015, according to the World Shipping Council. The ship emission has become one major air pollution source in the coastal and riverine areas of China. To our knowledge, field study has rarely been conducted, especially at emissions from CVs (coastal vessels) and RVs (riverine vessels) in China. Therefore, the characteristics of gaseous (CO, SO_2, NO, NO_2, NO_X, NMVOCs) and particulate matters (PMs, number and mass size distributions) emissions regularly sailing on the China East Sea and Yangzi river were investigated in this study. Effects of running condition (engine speed: 400~640 rpm) and fuel quality (HFO: 2.07% of fuel S, and MDO: 0.12% of fuel S) on gaseous and $PM_{2.5}$ emission factors from CVs and RVs were systematically compared.

The emission factors of NO_X, SO_2, CO, NMVOCs and $PM_{2.5}$ from RVs operated with MDO under different load conditions and CVs operated with HFO and MDO under same load conditions varied in the range of 50~80, 10~35, 8~23, 0.05~0.5 and 0.4~3.2 $g{\cdot}(kg\ fuel)^{-1}$. This study found that the emission of CO and NO_X were determined by engine (RVs and CVs) and its operating condition, while emissions of SO_2, NMVOCs and $PM_{2.5}$ were influenced by both fuel quality and engine operating condition. The particle number size distribution of in plumes of RVs were dominated by particles in the accumulation mode with peak at 70–90 nm, while the highest number concentrations increased from ~10^7 to ~10^8 cm^{-3} when the engine speed increased from 400 to 640 rpm at a 75% of full engine load. The mass ratio of fine particles ($PM_{2.5}$) in total suspended particles was about 82–87%. The $PM_{2.5}$ was dominated by organic carbon (OC) and elemental carbon (EC). The percentages of EC increase from 19% to 61% with increasing engine speed from 400 rpm to 640 rpm in 75% loads, while those of OC decrease from 51% to 23%. The variation of EC/OC percentages is owing to that an increase of engine speed results in increase of fuel usage and flue temperature, as well as decrease of air-to-fuel ratio. Additionally, the fractions of SO_4^{2-} exhibit much less variation with engine speed.

4CA.12

Comprehensive Assessment of Carbonaceous PM2.5 in Malaysia during Haze Events Influenced by Indonesia Peatland Fire and Non-Haze Period. KURITA HIROKI, Fujii Yusuke, Tohno Susumu, Saito Nozomi, Kamiya Yuta, Takayuki Kameda, Regina Hitzenberger, Haller Theresa, Ikeda Kazuhiro, Sakai Nobumitsu, Sulong Nor Azura, Mohd Talib Latif, Ohura Takeshi, *Kyoto University*

Biomass burning (BB) is one of the major sources of PM2.5 in Southeast Asia. Especially, haze from peatland fire in Indonesia frequently causes serious environmental problems such as human health impact, visibility impairment and regional climate change in ASEAN countries during dry season. Carbonaceous components are the dominant species of BB aerosols and their comprehensive characterization is indispensable to assess their effects on environment or conduct effective source apportionment. In this study, twenty four-hour PM2.5 filter samples were obtained by annual sampling in Kuala Lumpur, Malaysia (sampling site: 3° 8′ 20.4′′ N, 101° 41′ 12.6′′ E, 56 m above sea level) from June 2015 through May 2016 with a total of 139 samples. Detailed information of sampling site in this study has been provided in the previous report (Sulong et al., Sci. Total Environ., 601-602, 556-570, 2017). The samples were subjected to chemical analysis of elemental carbon (EC), organic carbon (OC), water-soluble organic carbon (WSOC), carbon content of humic-like substances (HULIS-C), polycyclic aromatic hydrocarbons (PAHs) and their derivatives, other biomass pyrolysis-derived compounds, and components of biogenic secondary organic aerosols (SOA). EC and OC were analyzed by a thermal-optical reflectance method with IMPROVE_A protocol. Black carbon (BC) and brown carbon (BrC) were also determined by an integrating sphere method (see Wonaschütz et al., Environ. Sci. Technol., 43, 1141-1146, 2009).

PM2.5 mass concentrations ranged from 7.4 to 241 μg m-3 with an annual average of 38.2 μg m-3. OC was the dominant component of PM2.5 and the concentrations varied from 1.3 to 40 μg m-3. EC concentrations were in the range of 0.3 to 6.1 μg m-3, while BC concentrations were from 0.22 to 2.4 μg m-3. There was significant discrepancy between EC and BC concentrations of the most samples collected in the peatland fire season (August – October), however, EC concentrations agreed well with those of BC during non-fire periods (June, July, and November – May). BC concentrations was virtually constant of around 2 μg m-3 for the samples whose EC concentrations were higher than 3 μg m-3, or concentrations of levoglucosan, a typical BB marker were higher than 0.5 μg m-3. This result suggests that higher concentrations of BB components have influence on the thermogram of the EC/OC analysis and contribute to the positive potential bias in EC determination resulting from the slipping of residual OC into the He/O2-mode and its potential evolution after the split point by maximizing the evolution and/or pyrolysis of OC at high temperature in the He-mode (Cavalli, F. et al., Atmos. Meas. Tech., 3, 79-89, 2010). Effect of HULIS-C is also discussed. We have quantified 20 PAHs, 35 nitro-PAHs (NPAHs), 20 oxygenated PAHs (OPAHs) and 20 chlorinated PAHs (ClPAHs) in PM2.5. Annual average total concentrations of PAHs, NPAHs, OPAHs and ClPAHs were 1.37, 0.70, 1.19 and 0.037 ng m-3, respectively. Total concentrations of each PAHs showed remarkable increase for haze samples (PM2.5 concentration is larger than 100 μg m-3) compared with non-haze samples (PM2.5 concentration is less than or equal to 30 μg m-3). Regarding biogenic SOA tracers, β-caryophyllinic acid (β-caryophyllene ozonolysis product) concentrations of haze samples were much higher than those of non-haze samples.

4CA.13

Contrasting Temporal and Spatial Variation of Atmospheric Carbonaceous Aerosols during a Year-Long Measurement in Central India. SHAMSH PERVEZ, Rakesh Sahu, Suresh Tiwari, A.S. Panicker, Rajan K. Chakrabarty, Judith Chow, John Watson, Yasmeen F. Pervez, *Pandit Ravishankar Shukla University, Chhattisgarh, India*

Air pollution is now serious health concern in developing countries including India and has been responsible for adverse effects on human health. The study, presented here, describe the spatiotemporal variability in year-long measurements of ambient $PM_{2.5}$ and associated component of carbonaceous matter in rural, industrial and urban environments of Central India during October 2015 to September 2016. Weekly $PM_{2.5}$ aerosols sampling were carried out (gravimetrically) using a set of two parallel $PM_{2.5}$ cut-off impactors consisted MiniVol air samplers, positioned in an urban, industrial and rural environments of Raipur, Bhilai and Kosmarra (a village of Dhamtari District), Chhattisgarh, India. Urban site was also used to measure day and night time ambient $PM_{2.5}$ to evaluate the impact of meteorological parameters on occurrences of $PM_{2.5}$ masses. $PM_{2.5}$ deposited on quartz filters were analyzed for temperature resolved fractions of carbonaceous matter using Thermal/Optical carbon analyzer (DRI Model 2001) by following IMPROVE_A Protocol. The annual average $PM_{2.5}$ mass concentrations of rural, urban and industrial sites found to be ~2 to 5 folds higher than the Indian National Ambient Air Quality Standard (NAAQS). Higher occurrences of OC and EC in $PM_{2.5}$ was observed in the winter season, compared to those measured in the summer and post-rainy. Similarly, OC and EC concentrations were found to be higher at night time than those observed for daytime in the urban site. On comparing with reported values for other Indian locations, Raipur (urban) and Bhilai (urban-industrial) sites have shown the highest percentage of Total Carbonaceous Aerosols (TCA) in ambient $PM_{2.5}$. The annual mean ratio of OC/EC has been found to be 3.50 ± 1.76 (range 2.16 to 7.84) and 3.94 ± 0.98 (range 1.63 to 5.42) in urban and rural sites, respectively; indicates the dominance of biomass burning (BB) and incomplete combustion (IC) in industrial processes in occurrence of higher carbonaceous aerosols in ambient air. The average char/soot ratios are observed to be 3.65 ± 2.65, 1.77 ± 0.98 and 1.93 ± 0.62 for urban, rural and industrial sites, respectively. Contribution of secondary organic aerosol (SOA) to ambient OC and thermal fractions of OC and EC have also been investigated for rural, industrial and urban sites and analysis is in progress. The details results will be presented during the conference.

4CA.16

Metrology for Light Absorption by Atmospheric Aerosols: The EMPIR Black Carbon Project. Eija Asmi, Joel Corbin, Volker Ebert, Konstantinos Eleftheriadis, François Gaie-Levrel, Martin Gysel, Thomas Müller, Andreas Nowak, Konstantina Vasilatou, Ernest Weingartner, PAUL QUINCEY, *NPL*

Black carbon (BC) is widely recognized as the foremost particulate absorber of solar radiation in the atmosphere and has been associated with the detrimental health effects of air pollution. To monitor BC concentrations, the atmospheric-science community has developed an array of technologies based on light absorption measurements. These absorption measurements are typically reported as mass concentrations of Equivalent Black Carbon (EBC) by using a standard mass absorption cross-section at a given wavelength. However, there is currently a lack of SI traceability for such absorption measurements. In addition, the most common field instruments measure EBC after depositing aerosol particles onto a filter, which introduces complex uncertainties and a need for standardized calibration methods.

The EMPIR Black Carbon project, *Metrology for light absorption by atmospheric aerosols (2017 – 2020)*, aims to establish SI traceability for atmospheric aerosol light absorption measurements, based on filter-free methods such as extinction-minus-scattering, photoacoustic spectroscopy, or photothermal interferometry, as well as standardised calibration routines for filter-based instruments. To this end, its specific objectives are to (1) develop a traceable and primary method for measuring aerosol absorption at specific wavelengths, with defined uncertainties and (2) recommend well-characterized reference aerosols suitable for challenging filter-based instruments. Further co-benefits of this work are (3) the establishment of a set of well-defined physical parameters for the traceable quantification of EBC concentrations and (4) the development of a validated method for the in-situ calibration of filter-based field instruments.

This presentation aims to motivate and summarize the goals of the EMPIR project, which is currently in its early stages, in order to encourage and invite contributions from the community.

4CA.17

Usefulness of Stable Carbon Isotope and Other Chemical Tracers to Distinguish between Primary and Secondary Carbonaceous Sources of PM2.5 Particles over a National Park in Central India. SHILPI SAMIKSHA, Ramya Sunder Raman, *Indian Institute of Science Education and Research, Bhopal*

Carbonaceous aerosols were investigated by measuring the stable carbon isotopic ratio, $\delta^{13}C$ in bulk $PM_{2.5}$ particles. In this study, ambient $PM_{2.5}$ samples were collected over Van Vihar National Park in Bhopal, central India over a period of two years (01 January, 2012 to 31 December, 2013). 12 hour integrate samples were collected on to Teflon, Nylon, and quartz fiber filter substrates. Punches of the quartz fiber filters were analyzed for organic and elemental carbon (OC/EC) using a thermal-optical-transmittance/reflectance (TOT-TOR) analyzer operating with a 632 nm laser diode.

Punches of the quartz filters were further analyzed for concentrations of total carbon (TC) and their $\delta^{13}C$ were measured using elemental analyzer (Flash 2000) interfaced to isotope ratio mass spectrometer (EA-IRMS). The CO_2 produced was introduced into a MAT 253 isotope ratio mass spectrometer (IRMS) via a Conflo IV interface to determine the carbon isotopic ratio. Standard (Acetanilide and CH-3 cellulose) were measured after every 4 samples and every tenth sample was analyzed in duplicate. Duplicates were analyzed such that they covered the entire concentration range of the samples. A routine precision of ~ ± 0.1‰ was obtained.

This study will present preliminary results on the seasonal variations $\delta^{13}C_{TC}$ in $PM_{2.5}$ particles collected over the study site. We also investigate the relationships between $\delta^{13}C_{TC}$ concentration and the concentrations of other chemical tracers (mono and di-carboxylic acids, K^+), their seasonal variations, and associations with air parcel back trajectories. These relationships will be used to estimate the relative importance of primary and secondary organic aerosols at the study location. Further, isotope-mixing models (e.g., ISOSOURCE) will also be used for organic aerosol source characterization.

4CA.18

Source Apportionment of Fossil Fuel and Biomass Burning Black Carbon (Bc) in the Milan Metropolitan City and Bareggio Sub-Urban Area Contrasting Locations. AMIRHOSEIN MOUSAVI, Mohammad Sowlat, Ario Ruprecht, Constantinos Sioutas, *University of Southern California*

In the current work, spatial and temporal variation of black carbon (BC) were evaluated at two sites, including Milan, a metropolitan area primarily impacted by urban emissions, and Bareggio, a sub-urban area, from July to October 2017. Using the Equivalent Black Carbon (EBC) model, sources of BC were apportioned using the BC measurement data from seven-wavelength (AEE33) and two-wavelength (AEE51) aethalometers for Milan and Bareggio, respectively. Result indicated that BC concentrations are ranging from 0.75-1.65 $\mu g.m^{-3}$ in Bareggio with a peak in July and 1.05-1.56 $\mu g.m^{-3}$ in Milan with the highest values in October. In addition, MAC values for both 370 nm (7.2±0.6 $m^2.s^{-1}$) and 880 nm (16.2±0.8 $m^2.s^{-1}$) wavelengths showed a consistent temporal trend and between the sites with slightly higher values for Bareggio. Moreover, fossil fuel combustion contributions to the total BC concentrations (ranging from 72% in Bareggio to 96% in Milan) are relatively higher than those of biomass burning (ranging from 10% in Milan to 26% in Bareggio). For fossil-fuel-originated black carbon (BC_{ff}), major peaks were observed during the traffic rush hours, whereas the contribution of black carbon that originated from biomass burning (BC_{bb}) was maximum during nighttime reaching values as high as 25-30% of total BC concentrations in Bareggio site. Moreover, results of the ongoing measurements for the cold season of the study will also be presented to compare the levels and BC_{ff}% and BC_{bb}% across different seasons.

4CA.19

Wintertime PM2.5 in the Kathmandu Valley and Terai Region of Nepal. MD. ROBIUL ISLAM, Nita Khanal, Khadak Mahata, Siva Praveen Puppala, Narayan Babu Dhital, Michael Giordano, Benjamin Werden, Anobha Gurung, Arnico Panday, Peter DeCarlo, Elizabeth Stone, *University of Iowa*

Airborne particulate matter (PM) adversely impacts human health through respiratory and cardiopulmonary diseases. Kathmandu Valley and the Indo-Gangetic Plain (IGP) are experiencing serious PM pollution problems. PM pollution in these regions is worse in the winter months (December – February) when regional haze or "fog" events occur. This poster will present preliminary results from the second Nepal Ambient Monitoring field campaign on the levels, composition, and sources of $PM_{2.5}$ and PM_{10} in the Kathmandu Valley and in northern IGP during wintertime. PM samples were collected at Ratnapark (in the Kathmandu Valley at 1300 m a.s.l.), Dhulikhel (east end of the Kathmandu Valley at 1600 m a.s.l.), and Lumbini (in the northern IGP at 100 m a.s.l.) for 7-10 days at each site. The samples were collected during daytime and nighttime periods spanning December 20, 2017 - January 27, 2018. PM mass concentrations were determined and chemical analysis were conducted includes to determine levels of organic carbon (OC) and elemental carbon (EC), water soluble inorganic ions, and organic species. Organic speciation focused on molecular markers (a chemical species that is specific to an aerosol source) to gain insight to the sources of organic aerosol (i.e. biomass burning, garbage burning, fossil fuel combustion, secondary organic aerosol, etc.). These data will be used for the purpose of identifying primary and secondary sources of PM and to estimate source contributions to $PM_{2.5}$ and OC through chemical mass balance (CMB) source apportionment.

4CA.20

Measurement of Speciated Gaseous and Particulate Organic Nitrates in Urban Atlanta using FIGAERO-HR-ToF-I-CIMS.

MASAYUKI TAKEUCHI, Gamze Eris, Taekyu Joo, Yunle Chen, Weiqi Xu, Dao Huang, Gabriela Saavedra, Seongshik Kim, Dong Gao, Rodney J. Weber, Yele Sun, Michael Walker, Brent Williams, Jenna Ditto, Drew Gentner, David Tanner, Greg Huey, Nga Lee Ng, *Georgia Institute of Technology*

Owing to the semi-/low-volatile nature of organic nitrates and their implication for the budget of reactive nitrogen species (i.e. NO_x) and ozone formation, atmospheric organic nitrates have been receiving increased attention in the atmospheric research community. Previous field studies using online instruments, such as Thermal-Dissociation Laser-Induced Fluorescence (TD-LIF) and Aerosol Mass Spectrometer (AMS), have demonstrated the ubiquitous presence of organic nitrates across different continents and in different environments. However, there is limited understanding at the molecular level of such organic nitrate species and the seasonal effect on their chemical composition. Additionally, the dominant source (e.g. daytime vs. nighttime, primary vs. secondary, etc.) and the fate of organic nitrates are not well understood. In this study, the Filter Inlet for Gases and AEROsols (FIGAERO) coupled to High Resolution Time-of-Flight Iodide Chemical Ionization Mass Spectrometer (HR-ToF-I-CIMS) was used to measure speciated gaseous and submicron particulate organic nitrates at the Jefferson Street site in Atlanta, GA, USA which is an urban site in the Southeastern Aerosol Research and Characterization (SEARCH) network, using. Measurements were conducted in summer 2017 and winter 2018. Preliminary results show that C_{4-5} and C_{8-10} organic nitrates represent a significant fraction of total organic nitrates in summer, suggesting the important role of biogenic volatile organic compounds such as isoprene and monoterpenes. However, C_{8-10} organic nitrate species dominates over C_{4-5} organic nitrates in winter due to reduced isoprene emission. In addition, we observed high molecular weight compounds, tentatively assigned as C_{20} organic mono-/di-nitrates, in the particle-phase that exhibit a clear diurnal pattern peaking little after midnight. These high molecular weight compounds are also detected in laboratory chamber experiments of monoterpene NO_3 oxidation, implying a significant contribution of NO_3 chemistry to the formation of particulate organic nitrates in winter. Bulk volatility distributions of ambient organic nitrates derived from FIGAERO thermogram data are presented and compared with those of laboratory-generated organic nitrate aerosols to confirm the contribution of NO_3 oxidation to organic nitrate aerosol formation. Lastly, the effects of ambient temperature, relative humidity, NO_x level, and the level of various volatile organic compounds on the ambient concentrations of speciated and bulk organic nitrates will be discussed.

4CA.21

Measurements of Dry and Wet Black Carbon Deposition over a Grassland. GAVIN MCMEEKING, Ethan Emerson, Joseph Katich, Joshua P. Schwarz, Delphine Farmer, *Handix Scientific*

The atmospheric lifetime of black carbon (BC), an important light-absorbing aerosol component, is controlled by wet and dry deposition, which are poorly constrained by observations. We apply a single particle soot photometer (SP2), which measures the mass of refractory BC in particles using laser-induced incandescnce, to measure surface-atmospheric exchanges of BC via eddy covariance. Measurements were performed at the DOE ARM Southern Great Plains site in Oklahoma during summer. Wet deposition measurements of BC were also performed by analyzing collected precipitation samples through a combination of nebulization followed by SP2 measurement. We report on the relative importance of dry and wet deposition processes during the study, and estimate a BC lifetime with respect to each process. Additional eddy covariance measurements performed in other locations are also discussed.

4CA.24

Equivalent Black Carbon (EBC) Measurement at a Regional Background Site in Central Europe Using a Multiple Wavelength Aethalometer: Variability and Source Apportionment. SALIOU MBENGUE, Norbert Serfozo, Jaroslav Schwarz, Nadežda Zíková, Adéla Holubová Šmejkalová, Ivan Holoubek, *Global Change Research Institute, CAS, Brno 60300, CZ*

Equivalent Black carbon (EBC) is a primary carbonaceous aerosol emitted from a variety of combustion related sources. It is recognized to play an important role on adverse public health and in the Earth's climate system. Although measurements at background areas are important for better characterizing and understanding the influence of anthropogenic emissions on climate forcing and health effect, scarce studies have been reported in Eastern Central Europe using real-time EBC measurements. This study focuses on the seasonal, diurnal and weekly trends of EBC at a regional background site in Central Europe. Our aim is to identify the potential sources of EBC, especially the influence of fossil fuel and biomass burning.

The EBC in PM_{10} was monitored at NAOK (National Atmospheric Observatory Košetice, 49°35'N, 15°05'E), central Czech Republic. Measurements were performed from 2012 to 2017 at ground base (4 m) with a 5 min time resolution using a seven wavelength aethalometer (Model AE31, Magee Scientific). The EBC data have been corrected for loading effect, and Delta-C variable (EBC370nm-EBC880nm) was calculated.

Preliminary results show that concentrations of EBC are higher in winter than in summer, which could be related to the variability in sources intensities and meteorological conditions. The wavelength dependence of light absorption by collected aerosols will be investigated to identify the potential sources of EBC at the rural site. The diurnal cycles of EBC in the near-ultraviolet (370 nm) and in the near-infrared (880 nm) spectral regions are compared for winter and summer. The diurnal cycles are stronger in winter than in summer with lower concentrations observed at noon time when the mixing height reaches a peak (i.e. higher dispersion of pollutants). In summer, EBC emission could be mostly attributed to fossil fuel combustion, which is consistent with the smaller difference between diurnal profiles of λ_1 and λ_6. Delta-C values, a proxy for biomass burning is more pronounced in winter, which is consistent with the increased emissions from wood burning.

Furthermore, correlations will be examined between EBC and other parallel measurements of atmospheric pollutants (OC/EC, CO, $_{NO2,}$ SO_2) at NAOK. The influence of fossil fuel and biomass burning will be investigated deeper using Ångström absorption exponent and Delta-C.

4CA.25

Estimating Aerosol Light Absorption from Filter-based Spectrophotometer Measurements. APOORVA PANDEY, Nishit Shetty, Rajan K. Chakrabarty, *Washington University in St Louis*

Filter-based instruments, such as the aethalometer, particle soot absorption photometer and UV-vis spectrophotometer, estimate aerosol light absorption by measured attenuation through an aerosol loaded filter. The conversion of attenuation coefficient to absorption coefficient is subject to several measurement artifacts, including multiple scattering of light by the filter and "shadowing" effects from increasing loading of aerosols. In general, the magnitude of these artifacts depends on the properties of the filter substrate, the aerosol optical loading, and the aerosol single scattering albedo (SSA). The relationship between aerosol light absorption and filter based transmittance or reflectance measurements needs to be established for each instrument and filter substrate combination. In this work, we evaluate the use of Teflon membrane filters in a UV-visible spectrophotometer to estimate absorption coefficients. Particles with SSA values ranging 0.4-0.99 were generated using flaming/smoldering phase combustion of a variety of biomass types. Aerosol samples were collected on Teflon and quartz fiber filters in parallel with in situ measurements of absorption and scattering coefficients using multi-wavelength Photoacoustic Spectrometers with integrated nephelometers at 375, 405 and 532 nm. A high-resolution UV-vis spectrophotometer equipped with an integrating sphere was used to measure transmittance and reflectance spectra from the Teflon filters. An attenuation value was calculated using the above measurements. The ratio of the aerosol absorbance (calculated from photoacoustic measurements) and the filter attenuation is commonly designated filter correction factor; this factor was positively correlated with the attenuation (loading effect), but showed an inverse relationship with SSA. We found that for a wide range of aerosol properties (i.e. SSA), the absorbance can be conveniently expressed as a simple function of the attenuation measurements, with no need of additional parameters. The behavior of the aerosol-filter system was also modeled by applying the solution of two-stream model of radiative transfer in one dimension to a two-layer approximation of the system. The predicted relationship between absorbance and attenuation was consistent with the experimental data.

4CA.26

Brown Carbon Aerosol Observed in the Remote Atmosphere. LINGHAN ZENG, Rodney J. Weber, Aoxing Zhang, Yuhang Wang, Eric Scheuer, Jack Dibb, Jose-Luis Jimenez, Pedro Campuzano-Jost, Joshua P. Schwarz, Kathryn McKain, Eric Apel, *Georgia Institute of Technology*

Organic aerosols (OA) have long been thought to only scatter sun light and thereby cool the climate. However, a portion of organics, so called brown carbon (BrC) absorb strongly at shorter wavelengths. BrC is emitted by the incomplete combustion of fuels, especially biomass, or produced from secondary formation processes. BrC has been found to be ubiquitous in continental air masses. In both ambient and laboratory studies, as BrC ages, it is observed to become less effective as a light-absorber due to photo-bleaching effects. The global radiative impact of BrC is difficult to assess with models owing to the large uncertainties in its emissions and chemical processing in the atmosphere. Lack of global scale BrC data sets limits our understanding of BrC processing and precludes meaningful model simulation assessments. The NASA Atmospheric Tomography (ATom) mission provided an opportunity to make measurements of BrC in the remote atmosphere over global extents reaching near pole-to-pole along the central Pacific and Atlantic oceans during different seasons. During ATom, filters loaded with ambient aerosol sampled with the NASA DC-8 research aircraft were extracted into water and methanol, sequentially, and the light absorption of the solutes was determined via long optical path capillary measurements. The results provide the first data set of BrC on a global scale. Generally, BrC concentrations are found to be very low in most of the remote atmosphere, and detectible levels were only found in specific regions, including the mid-Atlantic downwind of African or South American fires and in regions of the Arctic. Further data analysis, including comparisons with predictions from the Community Atmosphere Model version 5 (CAM5) of the Community Earth System Model (CESM) are used to better understand the sources, atmospheric loss and transport processes, and radiative impacts of BrC on a global scale.

4CA.27

Fourier-transform Infrared Determination of Organic and Elemental Carbon: Anomalous Samples and What They Tell Us about Composition and Sources. ANN DILLNER, Andrew Weakley, Bruno Debus, Satoshi Takahama, *University of California, Davis*

Several studies have demonstrated that thermal optical reflectance (TOR) OC and EC in fine aerosol can be predicted from Fourier transform infrared (FT-IR) spectra of aerosol samples collected on polytetrafluoroethylene (PTFE) filters. Calibrations for OC and EC are developed using partial least squares regression and provide equivalent OC and EC mass with accuracy and precision comparable to TOR. For most samples, one calibration model developed from samples from multiple sites is needed to predict OC and EC across sites and seasons. Here, we discuss cases in which multi-level modeling is needed for high quality predictions. For example, in the Chemical Speciation Network (CSN), which provides speciated particulate matter concentrations at urban sites, samples from one site with (presumably) distinctive EC sources are not well predicted by the calibration developed for all samples. To accurately predict EC on these anomalous samples, “ordinary” EC is distinguished from more “anomalous” EC using the sample’s FT-IR spectrum and a classification algorithm (partial least squares discriminant analysis). Samples collected from the Elizabeth, NJ sampler, located near a major tollway, often contained anomalous EC. Further analysis of FT-IR spectra and TOR fractions suggested that Elizabeth samples likely contained elevated levels of EC from fresh diesel exhaust as evidenced by the use of organic nitrogen functional groups for prediction, very low average OC/EC, and minimal charring during TOR speciation. FT-IR EC from the other eight sites in this study was predominately determined by aliphatic C-H, C=C aromatic, and functional groups associated with oxidation. Two calibration models were developed, one for ordinary and one for anomalous spectra. Classified spectra were allocated to their associated calibration resulting in a significant reduction in prediction error (30% to 21%; $p<0.05$). This study provides insights into appropriate tools for accounting for significantly different chemical compositions at different sites and into the character of carbonaceous aerosol at heavily diesel impact sites as compared to more typical urban environments. Additional examples from the Interagency Monitoring to Protect Visual Environments (IMPROVE) network will be presented.

4CA.28

Particulate and Gas Phase Separation in Simultaneous Sampling of Combustion Byproducts: New Insights into Chemical Composition by Mass Spectrometric Analysis. Jennifer Noble, Linhdan Ngo, Dumitru Duca, MARIN VOJKOVIC, Abd Raouf Ikhenazene, Cornelia Irimiea, Guillaume Lefevre, Alessandro Faccinetto, Claire Pirim, Yvain Carpentier, Bertrand Chazallon, Nicholas Nuns, Jerome Yon, Eric Therssen, Cristian Focsa, *Université de Lille*

Combustion is the largest anthropogenic source of aerosol particles, accompanied by significant gas phase byproducts. Combustion soot particles can have a direct or indirect effect on climate that gives rise to important consequences for both atmospheric radiative forcing and cloud formation and lifetime. Although many studies have been conducted to characterise soot particles (e.g. Parent et al. 2016), more extensive investigation of their composition and molecular structure is required in order to better understand the role of particulate and gas phase combustion byproducts in atmospheric physicochemical processes.

In this study, a new simultaneous sampling method was developed for combustion byproducts in the particulate and gas phases. The experimental protocol was verified using a Combustion Aerosol Standard (CAST) burner supplied with various propane-air mixtures. Combustion byproducts were collected on two quartz microfibre filters in series. Firstly, a “front filter” was used to collect particulate matter and, secondly, a “back filter” covered with carbon black adsorbed gases that passed through the front filter, following the principle of Faccinetto et al. (2011).

An analytical approach combining micro-Raman and micro-Fourier Transform Infrared spectroscopies with Secondary Ion Time-of-Flight Mass Spectrometry (ToF-SIMS) and Two-step Laser Mass Spectrometry (L2MS) was adopted, in order to characterise the structural and chemical properties of the sampled particulate and gas phases. The custom built L2MS setup allows a detailed chemical analysis of trace amounts of deposited particles at the molecular level, revealing the presence of chemical classes such as aliphatics, aromatics, nitrogenated- /oxygenated-hydrocarbons, organosulfates and metals. For combustion soot, the degree of aromaticity, determined by the relative abundance of polycyclic aromatic hydrocarbons (PAHs), is decisive in determining its physicochemical properties. The L2MS technique is especially well adapted for PAH detection. ToF-SIMS has high sensitivity for both inorganic and organic species, notably the Cn- ion series, a proxy for elemental carbon. Vibrational spectroscopies provide complementary information about the chemical composition and structure of soot by probing the vibrational modes of its composite molecules (Ess et al. 2016).

Our combined mass spectrometry and vibrational spectroscopy studies suggest that the gas and particulate phases of combustion byproducts are sampled effectively using the chosen methodology, and confirm that they have significantly different chemistry. In the samples used to validate the method, the mass distribution of PAHs is found to vary significantly, not only with operation point of the CAST burner but also between the gas and particulate phases. Principal component analysis allowed discrimination between different working points of the burner, in both the particulate and gas phases. The gas phase of all sampled working points contains lower mass PAHs than the particulate phase and, perhaps surprisingly, the mass distribution of gas phase PAHs varies with the richness of the fuel-air mixture.

Following successful validation of the sampling and analysis protocol, combustion byproducts were sampled with the same double-filter method in a kerosene flame (with direct interest for the aeronautical domain). We present a comparison between CAST and flame byproducts in the particulate and gas phases.

This work was supported by the French National Research Agency (ANR) through the PIA (Programme d'Investissement d'Avenir) under contract ANR-10-LABX-005 (CaPPA – Chemical and Physical Properties of the Atmosphere), the European Commission Horizon 2020 project PEMs4Nano, and the CLIMIBIO project via the Contrat de Plan Etat-Région of the Haut-de-France region.

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[2] Faccinetto, A., Desgroux, P., Ziskind, M., et al. (2011) Combust. Flame 158, 227-239.
[3] Parent., P., Laffon, C., Marhaba, I., et al. (2016) Carbon 101, 86-100.

4CA.29

Apportionment of Black Carbon to Fossil Fuel and Biomass Burning Sources in the Lower Fraser Valley, British Columbia: Impact of 2017 Wildfires on Local Air Quality. Robert Healy, Geoff Doerksen, UWAYEMI SOFOWOTE, Yushan Su, Jerzy Debosz, Michael Noble, Cheol H. Jeong, Jon M. Wang, Nathan Hilker, Greg J. Evans, Anthony Munoz, *Ontario Ministry of the Environment and Climate Change*

One year Aethalometer datasets collected concurrently at six sites in the Lower Fraser Valley, British Columbia from September 2016 through August 2017 have been analyzed in order to investigate the relative importance of fossil fuel and biomass burning contributions to black carbon (BC) in the region. The sampling sites are located in North Vancouver, Richmond, South Burnaby, Port Moody, Abbotsford and Chilliwack. These sites experienced annual mean BC mass loadings in the range 0.3-0.7 $\mu g\ m^{-3}$, with the highest concentrations observed in Vancouver and the lowest in Chilliwack, a small city located approximately 100 km east of Vancouver. BC was apportioned to fossil fuel and biomass burning sources at hourly resolution using the dual-wavelength optical model approach, first incorporating assumed alpha values of 0.90 and 2.09, respectively. However, applying a value of 2.09 was found to significantly underestimate the fraction of BC from biomass combustion (BC_{bb}) during a prolonged wildfire smoke event which persisted for 10 days in August 2017 and impacted air quality severely in the region. Hourly resolution $PM_{2.5}$ concentrations in excess of 100 $\mu g\ m^{-3}$ were recorded several times at multiple sites during this event and mean ambient $PM_{2.5}$ concentrations for the 10 day period were up to eight times higher than mean concentrations for the remainder of the summer. Using a difference approach to estimate the BC mass associated with the wildfire plume enabled an optimization of the alpha value for wildfire aerosol at each site. Similar wildfire alpha values were determined at all six sites using this approach 1.40 ± 0.10, which is sensible considering that all sites were influenced simultaneously by the same plume. The highest hourly resolution wildfire BC_{bb} mass loadings were observed at Chilliwack (7.3 $\mu g\ m^{-3}$), which is situated closest to the wildfire source regions, identified using conditional probability function and quantitative transport bias analyses. For the Lower Fraser Valley sites investigated, approximately 34-45% of total summertime exposure to BC and 64-86% of total summertime exposure to BC_{bb} occurred during the 10 day wildfire event. On an annual scale, however, residential wood combustion is estimated to be a larger contributor to ambient BC than wildfires at every site.

4CA.30

Source Apportionment and Variability of Submicron Organic Aerosol from Year-long Near Real-time Measurements Over an Urban Mediterranean Area. Aikaterini Bougiatioti, IASONAS STAVROULAS, Despina Paraskevopoulou, Georgios Grivas, Pavlos Zarmpas, Eleni Liakakou, Evangelos Gerasopoulos, Nikolaos Mihalopoulos, *National Observatory of Athens*

Organic aerosol (OA) represents a large fraction of submicron aerosols worldwide, especially in urban areas. During the winter season, wood combustion is one of the major sources of OA in Europe (Puxbaum et al., 2007) which apart from contributing to the production of primary aerosol, is also responsible for significant secondary organic aerosol formation (Heringa et al., 2011). The economic recession in Greece during the past seven years has caused a deceleration of industrial activity and limitation of vehicular circulation (Paraskevopoulou et al., 2014). Strong correlation between economic indicators and several pollutants levels, reveal that this recession has resulted in significantly lower levels of pollutants in many large cities of Greece (Vrekoussis et al., 2013). Nevertheless, this crisis has lead residents to the “cheaper” solution of uncontrolled wood and biomass burning for domestic heating purposes, causing significant air quality deterioration. During summer all concentration levels are significantly lower and sources are more regional than local.

This study focuses on high temporal resolution chemical composition measurements performed in downtown Athens during three different winter periods and also a complete year, in order to identify the different sources of organic aerosol seasonally. It occurs that overall, organic aerosol represents half or even more of the total PM1 mass, with concentrations during all studied winters reaching up to 240 μg m-3. During the cold period 5 different factors of OA are identified, namely hydrocarbon-like OA (HOA), contributing an average of 15%, cooking OA (COA) with 9% contribution, biomass burning OA (BBOA) with 12%, a highly oxidized, low volatility OA factor (LV-OOA) with 34% and a semi-volatile OA (SV-OOA) contributing the remaining 30%. This SV-OOA has high affinity with biomass burning tracers, denoting its provenance from the fast oxidation of primary combustion sources. If the provenance of SV-OOA is combined with the primary BBOA and primary HOA from central heating systems, it is clear that almost half of the organic aerosol during wintertime in Athens originates from combustion activities.

During the warm period, 4 different factors of OA are identified, the same as before except for the primary BBOA. HOA contributes around 5.5% to the total organic fraction, COA 12%, SV-OOA around 38% and the rest 44.5% is attributed to LV-OOA. SV-OOA during summertime may be derived either from the oxidation of primary COA or from biogenic sources. Nevertheless it is clear that during the summer period the prevailing source of OA is the much oxidized OA, which has a more regional character and is linked to secondary aerosol formation.

Backtrajectory analysis, using the Potential Source Contribution Function (PSCF) method, and combination of pollutant concentrations with wind direction and speed, through Non-Parametric Wind Regression techniques were applied, in order to determine the local or regional origins of atmospheric pollution in downtown Athens throughout the year.

4CA.31

Impact of Organic Aerosol Partitioning on U.S. Particle Emission Factors. BENJAMIN MURPHY, Christos Efstathiou, Havala Pye, *United States Environmental Protection Agency*

Direct emissions of particulate-phase organic and inorganic compounds contribute the majority of near-field particle mass from combustion sources, especially in urban areas. For sources with substantial organic fractions (e.g. vehicles, fires, power plants, etc), previous studies have demonstrated the importance of considering reversible partitioning of organic compounds between the gas- and particulate-phases when linking laboratory/field measurements with predictions of ambient concentrations, from e.g. chemical transport models (see e.g. Murphy et al., 2017). For example, studies that characterize the emission factors or composition of particles from specific sources may be performed at much higher concentrations than what is relevant for the atmosphere and their emission factors must be adjusted to take nonlinear evaporation processes into account.

Any of several potential pitfalls could occur when combining emission factor databases (e.g. National Emissions Inventory, NEI), speciation databases (e.g. SPECIATE), emission models (e.g. MOVES, SMOKE) and chemical transport models (e.g. the Community Multiscale Air Quality model, CMAQ). These include how one corrects for adsorbed and absorbed vapors from the experiment, and how one applies distributions in volatility from literature in order to calculate the effects of partitioning on the pollutant phase distribution. Due to the complexity and enormity of these databases/models and the limited reporting from many of the studies that inform these systems, a comprehensive evaluation of these uncertainties is difficult.

We bridge the gaps between emissions inventories and models by reviewing the most important sources for direct organic particle emissions in the U.S. We then apply the updated emissions scale factors directly in CMAQ and assess their impact on policy analyses. Finally, we recommend revisions to the inventories and emissions models so that transport models best reproduce the emission magnitudes and trends that have been constrained by focused lab/field studies.

Murphy et al, ACP, https://doi.org/10.5194/acp-17-11107-2017, 2017.

4CA.32

Long-Term Assessment of Sunset OC/EC with Chemical Speciation Network Measurements. STEVEN G. BROWN, Elizabeth Landis, Hilary Minor, Theresa O'Brien, Joann Rice, *Sonoma Technology, Inc*

As part of a U.S. Environmental Protection Agency (EPA) project to evaluate the feasibility of the Sunset Semi-Continuous Organic and Elemental Carbon (OC/EC) monitor, EPA sponsored the deployment of this monitor by local air quality agencies in Chicago, Illinois; Houston, Texas; Las Vegas, Nevada; St. Louis, Missouri; Rubidoux, California; and Washington, D.C. Sunset monitors were collocated with existing 24-hr measurements of OC and EC made via filter sampling as part of the EPA's Chemical Speciation Network (CSN); at Houston, St. Louis, and Washington, they were also collocated with Aethalometer instruments, which measure black carbon (BC). Sunset data were compared to CSN and Aethalometer data to assess whether the Sunset monitors could be deployed in a routine monitoring network application in lieu of instruments that make filter measurements. Agencies encountered significant operational issues with the Sunset monitors, substantially reducing the number of valid data points for the multi-year deployment. After screening for these issues, and excluding results that were suspect, we found that Sunset OC generally compared well with the CSN OC (r2=0.73 across five sites); the Sunset/CSN OC ratio was on average 1.06, with a range among sites of 0.96 to 1.12. Sunset thermal EC and CSN thermal EC did not compare as well, with an overall r2 of 0.22, possibly because 26% of the hourly measurements were below the Sunset EC detection limit. Sunset Optical EC had a much better correlation to CSN thermal EC (r2=0.67 across all sites), with an average Sunset/CSN EC ratio of 0.90 (range of 0.7 to 1.08). There was also a high correlation of Sunset Optical EC with Aethalometer BC (r2=0.77 across all sites), though with a larger bias (average Sunset/Aethalometer ratio of 0.56). There was no systematic difference among the measurements by site location, i.e., Sunset Optical EC was consistently lower than Aethalometer BC at all three sites, with no significant seasonal variation. Collocated Sunset instruments at St. Louis had high precision, with r2 values of 0.93 for OC and 0.91 for Optical EC. Somewhat surprisingly, the diurnal pattern of OC was fairly invariant, while a morning peak was observed for EC at all sites. Overall, operational issues with the Sunset monitors were persistent at all sites, but when the instruments were operating well, collected data were comparable to results from the CSN and the collocated Aethalometers.

4CA.34

Effects of Sugarcane Pre-Harvest Burning on Aerosol Optical Properties in the Cauca Valley, Colombia. ANGELA VARGAS, Jennifer Marin, Lady Mateus, Nestor Rojas, Rodrigo Jimenez, German Ruega, *Universidad Nacional de Colombia*

Open biomass burning increases the concentration of gaseous pollutants such as CH4, CO, SO2, NOX, VOCs, and Particulate Matter (PM), which contains trace metals, organic compounds, elemental carbon and ions. Pre-harvest burning in extensive sugarcane plantations is a significant source of elemental carbon and organic compounds, including highly carcinogenic and mutagenic polycyclic aromatic hydrocarbons (PAHs), which can be transported to urban centers.

Palmira, a city with 350,000 inhabitants in the Cauca river Valley, is surrounded by 238,204 Ha of sugarcane plantations and is the center of sugarcane–related agroindustrial activity. Health data show that its population suffers different diseases commonly related with air pollution, such as ischemic heart diseases (17%), cerebrovascular diseases (8%), chronic respiratory diseases (7%) and acute respiratory diseases (5%). Furthermore, the impact of pre-harvest burning emissions on local air pollution in Palmira has not been determined.

This work focuses on the analysis of physical and optical properties of aerosols in Palmira with the aim to estimate the impact of sugarcane pre-harvest burning on air quality. The sampling site is located at the National University of Colombia (3º30’44.2620” N, 76º,18’27.3960 W) on a building rooftop. A sun photometer CE-318 of AERONET network was used to measure long term the Aerosol Optical Depth (AOD) and Angstrom Exponent, furthermore a Nephelometer IN 101 of SPARTAN network to measure Total and Back scattering (Red, Green and Blue).

AOD values oscillated between 0.01 and 0.42, higher than AOD measured at large cities in Colombia. The Angstrom Exponent was 1.54, associated with fine particles. The aerosol size distribution shows two size modes, a fine mode around 100 nm and a coarse mode around 3 um. The preliminary data of sun photometer and nephelometer show relationship between AOD (500 nm) and Total scattering.

4CA.35

Measuring the Physical Properties of Refractory Black Carbon off the Los Angeles Coast. JOSEPH KO, Trevor Krasowsky, George Ban-Weiss, *University of Southern California*

Black carbon (BC) is widely known to impact the radiative balance of the atmosphere, subsequently playing a role in global climate. The physical properties of refractory black carbon (rBC) were measured using a single particle soot photometer (SP2) on Catalina Island between September 7 and September 14, 2017. Catalina Island is located off the coast of Southern California, approximately 22 miles southwest of the Port of Los Angeles. The mass concentration, number concentration, and coating thickness was analyzed in conjunction with local/regional meteorology to characterize rBC properties for different meteorological regimes in this semi-remote sampling location. The campaign-averaged mass and number concentrations were 0.04 µg/m^3 and 20 cm^{-3}, respectively. This is approximately an order of magnitude lower than what has been observed in recent studies for the Los Angeles basin. Using the leading-edge-only technique, we found that approximately 27% (±19%) of rBC particles were thickly-coated, which is close to the lower end of values from past aircraft measurements in Los Angeles and the upper end of previous ground measurements in Los Angeles. HYSPLIT back-trajectory analyses were used for approximate source characterization. Many large fires in the Pacific Northwest were coincidentally active during the time of the sampling campaign, and preliminary back-trajectories show a high probability of impact from these biomass-burning events. The potential for spikes in rBC measurements due to passing cargo ships is also assessed.

4CA.36

Evaluating Inter-seasonal Urban Environment-mixed Black Carbon-induced Radiative Effects over Eastern India.

SHUBHA VERMA, Shantanu Pani, Sanhita Ghosh, Sauvik Santra, *Indian Institute of Technology Kharagpur*

The abundance of absorbing aerosols during the pre-monsoon season, consisting of locally emitted black carbon (BC) and of dust transported from near-by and far-off region have been suggested leading to elevated atmospheric heating effect. Sensitivity experiments using state of the art aerosol-chemistry-climate models reveal impacts of prevalent absorbing aerosols during the pre-monsoon season on the monsoon precipitation over India. Since atmospheric BC concentrations peak close to major source regions thus giving rise to regional hot-spots, BC-induced radiative warming effect could be more significant on a local to regional scale than the global, which in turn can have strong implications for the regional hydrological cycle. It is difficult to quantify such effects at a finer resolution of the urban scale using large-scale chemistry-climate models due to their coarser resolution and inefficiency to simulate fine scale aerosol properties.

Long-term observations of BC aerosols encompassing all seasons in an urban atmosphere in eastern India provided a unique opportunity to quantify the inter-seasonal urban environment-mixed BC-induced radiative effects. Under an influence of inter-seasonal transport processes and season-specific anthropogenic activity, urban environment-mixed BC-induced radiative effects were evaluated in the vicinity of aerosol composition constituted of enhanced anthropogenic constituents during winter/northeast monsoon season and elevated dust storms during summer/southwest monsoon season. In the present study, we applied a receptor modelling approach to quantify these effects. This was done through the application of long-term simultaneous observations of BC in conjunction with the total aerosol concentration and aerosol optical properties in the configuration of aerosol optical and radiative transfer model. Modelling experiments were designed using this model to simulate urban environment-mixed BC-induced radiative effects.

Our study indicated while the surface BC concentration exhibited a large seasonal variability, the value of BC-AOD was consistently high throughout; except during southwest monsoon season when this value was lower by about three times than that during rest of the seasons. A considerable change in the net radiation balance and an enhancement in radiative forcing efficiency and the atmospheric heating rate was estimated when BC was mixed with atmospheric aerosol constituents compared to unmixed BC; seasonal mean radiative forcing efficiency values due to mixed BC was about 8 to 13 times the unmixed BC value at the top-of-atmosphere. The urban environment-mixed BC-induced radiative heating effect during summer was estimated being higher than during southwest monsoon by 13% only, compared to by a factor of two times during winter season. While the summertime mean value of radiative forcing efficiency was about two times, the southwest monsoon mean value of the same was five to seven times the value during winter at all layers of the atmosphere. Enhanced urban environment-mixed BC-induced net radiative warming effect inferred during summer and southwest monsoon season was found consistent with our postulate about the possible signatures of this estimated effect in real observations of seasonal surface temperature features. Our study thus suggests mitigation of BC emissions may not be sufficient to curb urban environment-mixed BC-induced warming effect under the prevalence of prominent dust transport; thus drawing attention towards the complex role of mitigation measures to reduce pollution-induced radiative effects and its impact on regional climate.

4CM.2

Engineering Controls to Reduce Exposure to Respirable Crystalline Silica during Stone Countertop Grinding.

CHAOLONG QI, Alan Echt, *NIOSH*

Natural and engineered stone countertops became increasingly popular among consumers in recent years. Unfortunately, a large amount of dust that contains crystalline silica can be produced during stone countertop fabrication and installation. Inhalation of respirable crystalline silica (RCS) is one of the best-documented workplace hazards, with a large body of research strongly demonstrating that chronic overexposures cause silicosis and increase the risk of lung cancer. Finishing stone countertops using handheld grinders was among the tasks with the highest exposures to RCS documented in a NIOSH Health Hazard Evaluation at a stone countertop factory, where the exposure levels exceeded the NIOSH Recommended Exposure Limit (REL), even during wet grinding with water supplied to the grinder. In this study, NIOSH researchers investigated two additional engineering control measures for reducing workers' exposures to RCS during stone countertop grinding: a mobile dust control booth where countertop grinding was done inside the booth, and a sheet-water wetting method in addition to the existing water-fed grinder. The effectiveness of these two engineering control measures was evaluated in a series of field surveys and the results are reported in this presentation.

4CM.3

Microwave-Assisted Catalytic Total Oxidation of Methyl Ethyl Ketone over Co3O4 Catalyst. QUI NGUYEN VAN, Ha Than Quoc An, Thanh Nguyen Dinh, *Institute of Applied Materials Science - VAST*

Methyl ethyl ketone (MEK) is commonly used as a solvent in several chemical processes, but now emissions of MEK to the atmosphere can lead to human health and wider environmental problems. A combination process of catalytic oxidation and microwave heating was employed to remove MEK over Co3O4 nanostructure catalyst. The results showed that MEK has been decomposed effectively at 325 ^{0}C. Compared to conventional heating, the microwave assisted catalytic reaction was enhanced by lowering the operation temperature and has had no decrease in the catalytic activity when the space velocity increased from 11000 to 22400 h^{-1}. The results reveal the advantage of microwave energy for the reaction. Co_3O_4 catalyst showed a high endurance against water vapor in stream of the reaction.

4CM.4

Effect of RH Change on Pressure Drop of Loaded Cellulose Filter Media with Hygroscopic Deposits.

CHENXING PEI, Qisheng Ou, David Y. H. Pui, *University of Minnesota*

Current air filter test methods load test filter with non-hygroscopic blends, primarily dust, thus the testing RH is not a big concern. However, hygroscopic particles, mainly salts, are important portion of the ambient air pollutant. It is worthwhile to study the hygroscopic particle loading properties of air intake filters. Our previous research found that the loading RH has an impact on the test filter holding capacities when the hygroscopic particles were loaded. However, those research loaded the test filter media at the constant RH, which is not real in applications. The RH may change rapidly in some scenarios, such as thunderstorms in hot summer would increase the RH from a certain percentage to 100%. For the loaded filter media, this kind of RH change would not only affect how pressure drop increases during the high RH period, but also have impact on the loaded hygroscopic deposits. In this study, we studied the impact of RH change on the loaded hygroscopic deposits. We used potassium chloride, ammonium sulfate, ammonium nitrate to load the test filter media separately. We first loaded the test filter media to 4 inch of water at X% RH, and stopped the atomizer while keeping the test filter face velocity constant. Then we changed the RH to Y% and stopped the test until the instantaneous pressure drop change rate was less than 0.1inch water/hr. The pressure drop was recorded during the test. The selected X% and Y% RH covers from below the salts' efflorescence RH to above their deliquescence RH, thus salts may experience the transition from dry state to wet state or the reverse transition. The final pressures were compared as a function of the X%, Y% RH and salt kinds.

4CM.5

Enhancing the Efficiency of Flat-plate Electrostatic Precipitator by a Diffusion Charge Method. Chih-Te Wang, Chang-Chin Chou, Yu-Chau Wang, Shui-Jen Chen, Ken-Hui Chang, WEN-YINN LIN, *Institute of Environmental Engineering and Management, NTUT*

Diffusion charging is one of the commonly used collection methods for electrostatic trapping of nano-particles (dp<100 nm). Diffusion charging can avoid the direct contact between charging electrode and volatile organic compound (VOC) in treating the waste air. Research has shown that diffusion charging is a practicable method, but there is little experimental evidence for the maximum value of charged particles after charging. Therefore, this research designed a diffusion charger and let the air flow though the charger to generate high concentration ions for particle charging. The factors that can influence particle charging contain ion concentration, particle diameter, and charging time. This research investigated the charge distribution of different particle diameter at various carry gas rate and voltage of diffusion charger. Finally, charged particles stream into flat-plate Electrostatic precipitator to investigate particle penetration at different carry gas rate and voltage. The experimental results indicated that particle charging efficiency, increased with increasing air flow rate and corona voltage of unipolar diffusion charger, The best charging efficiency occur when the corona voltage and air flow rate is 3.3 kV and 3 lpm, respectively. Moreover, 50 nm particle carries 3 elementary charge with ratio of 36.7%, and 100 nm particle carries 6 elementary charge with ratio of 38.9%. Moreover, particle penetration decreased with increasing airflow rate and corona voltage of unipolar diffusion charger, and penetration of nanoparticle was higher than that of submicron-particle (100 nm <dp<1000 nm). Because, the surface area of nanoparticles is too small, it is hard for nanoparticles to get enough charge, and be collected. Therefore, there are a larger proportion of nanoparticles can pass through the flat-plate Electrostatic precipitator, compared with submicron-particles. The diffusion charging method is a feasible method was carried out through an indication of effectiveness of the experimental result. It is adopted both removal of organic waste gas and environment that must avoid the risk of explosion.

4CM.6

Charge and Filtration Characteristics of Novel Porous Fibers. Chih-Te Wang, Shao-Tai Lee, Jia-Hong Wang, Shi Jia-Xi, Chih-Chieh Chen, WEN-YINN LIN, *Institute of Environmental Engineering and Management, NTUT*

Filtration is one of the common, economical and effective methods for removing particulate. The electrets of surface in the fiber can achieve low-pressure loss without affecting the efficiency of filtration due to their electrostatic attraction. Previous researches were pointed out that increasing the specific surface area of fiber can increase the charge. At the same time, there were studies that had porous or hollow properties of the fiber can increase the specific surface area. In this study, three kind fibers of smooth, hollow porous and notch porous were prepared by electrostatic spinning. Then, with the charge test, the three fibers were charged by corona discharge method. The results showed that the average surface voltages were -0.82 kV (smooth), -0.90 kV (hollow porous) and -1.10 kV (notch porous), respectively. The highest charge of the porous fiber is due to its high surface area. Besides, experiments on the filtration efficiency of three types of fibers were carried out. Among them, the decrease rate of the perforated fiber penetration rate of the notch porous was more remarkable than that of the smooth and hollow porous fiber. After charging, the average fiber efficiency of smooth fibers increased from 0.16 to 0.29, the hollow porous fiber increased from 0.20 to 0.39, and the groove porous fiber increased from 0.21 to 0.47. The results showed that the charging and filtration quality of the notch porous fibers were better than the smooth and hollow porous fibers. Excellent performances will allow for notch hollow fibers to be easily integrated in the future various industries.

4CM.7

A Novel Technique for Testing Filter Media Using Monodisperse Aerosol as a Function of Aerodynamic Diameter.

Simon Payne, Martin Irwin, Tyler J. Johnson, JONATHAN SYMONDS, *Cambustion*

The standard ISO29463:2011 method of testing filter media efficiency as a function of particle size uses a Differential Mobility Analyzer (DMA) to select particles by electrical mobility. Depending on the size range of the source aerosol, it is possible for larger particles than selected to pass through the DMA, due to multiple-charging induced by the particle charging process used prior to classification. This can affect filter efficiency measurements if not taken into account. In addition, most DMAs are size limited to less than 1 micron.

The Aerodynamic Aerosol Classifier (AAC, Tavakoli and Olfert, 2013) is an instrument which classifies particles by aerodynamic diameter instead of electrical mobility diameter. Because it does not require particles to be electrically charged, this mitigates the DMA multiple-charging artefacts previously described. Furthermore, the currently available version of the AAC can classify particles from 25 nm to over 6 µm. This paper explores substituting an AAC for the DMA usually used in ISO29463:2011 filter efficiency tests to mitigate the issues described above.

Samples of filter media from two different types of half-mask respirators were mounted in an in-line filter holder. In turn, both sodium chloride and dioctyl sebacate aerosol sources from a nebuliser were classified using an AAC, to provide a monodisperse aerodynamic size selected aerosol. The penetration efficiency of the filter media in response to the monodisperse aerosol was evaluated by comparing particle number concentrations measurements upstream and downstream of the filter media using a condensation particle counter (CPC). This process was repeated over an aerodynamic size range from 50 nm to 3 µm (the upper limit was limited by the maximum detectable particle size of the CPC). As a comparison, the AAC was replaced with a DMA, to conform with the method prescribed by ISO29463:2011 (although only up to 750 nm due to the size limitation of the DMA).

On equivalent diameter size axes, the penetration efficiency curves between the AAC and DMA methods are similar, except for classification sizes smaller than the peak size of the nebulised source aerosol. This difference is attributed to a significant number of the particles selected by the DMA having 2 or more charges, and thus being much larger than intended. Due to the fact that a large proportion of particles remain uncharged in a neutraliser, the transmission efficiency of the AAC was found to be 1.5 to 5.5 times higher than the neutraliser-DMA system. This high transmission efficiency could be useful for more exotic test aerosols available only in limited concentrations.

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4CM.9

Improving the Accuracy of PM2.5 Sampling with Chilled Teflon Filter. Krishna Kumar Shukla, Sneha Gautum, Te-Hsien Hsieh, Ziyi Li, Pei-Yun Shih, THI-CUC LE, Chuen-Jinn Tsai, *National Chiao Tung University, Taiwan*

Most of the ambient aerosol sampling and monitoring devices use filter media to capture particles (such as $PM_{2.5}$) after the size-selective pre-separators (such as well impactor ninety-six (WINS), or very sharp cut cyclone (VSCC)). Smart heaters are further used to condition the inlet aerosol temperature to avoid water vapor condensation in the aerosol monitors. Previous studies from our group (Liu et al., 2014) showed that the aerosol evaporation loss was occurred which reduced the aerosol mass concentration. An increment in the deviation was also observed with decreasing loaded particle mass and increasing ambient or conditioning temperature (Liu et al., 2015). The aim of the present study is to use a chilled filter sampler in which the aerosol stream before the filter holder was chilled to 4 ^{0}C after the aerosol was dried to a relative humidity (RH) of 24.5 ± 5.1% to improve the accuracy of $PM_{2.5}$ sampling. The observed test results from the chilled filter sampler showed that the evaporation loss of volatile species was effectively suppressed. However, the gravimetric weights of chilled filter samples were slightly heavier than the normal filter samples, which were quantified by using hydrophobic test particles, due to slight increase in the remained water content in the former. A thin layer of condensed water coated on the sampling particles was the key to reduce the evaporation loss. After correcting the mass concentration of $PM_{2.5}$ for the excess remained water content, the accuracy of $PM_{2.5}$ sampling was greatly improved with the average positive bias reduced substantially from 15.2% to 2.6% for $PM_{2.5}$ ranging from 10.6 to 44.5 $\mu g/m^3$.

Keywords: aerosol sampling, evaporation loss, aerosol conditioning, $PM_{2.5}$ sampling inlet, aerosol instrumentation

Reference:

Liu, C.-N., Lin, S.-F., Tsai, C.-J., 2014. Sampling and Conditioning Artifacts of $PM_{2.5}$ in Filter-based Samplers, Atmos. Environ., Vol. 85:48-63.

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4CM.10

Improvement of Monitoring of Radioactive Aerosols of Ground-Level Air near Chernobyl NPP. ALEXANDR KALYNOVSKYI, Victor Krasnov, Boris Ogorodnikov, *Institute NSP NPP, Ukraine*

In order to control a work safety in areas erection of new safe confinement "ARKA" construction and staff's location near Chernobyl NPP (ChNPP) the radioactive aerosols (RA) of ground-level air were monitored. Sampling of aerosols was carried out by pumping air through filters FPP-15-1.5 which had area about 0.8 m^2. Average filtration rate was 8 - 12 000 m^3/day. The consist and activity of radionuclides in aerosols was determined by gamma spectrometer (CANBERRA). The concentration of ^{137}Cs was varied within $1.1 \cdot 10^{-4}$ - $2.3 \cdot 10^{-1}$ Bq/m^3, ^{154}Eu - $2.8 \cdot 10^{-7}$ - $1.4 \cdot 10^{-3}$ Bq/m^3, ^{241}Am - $1.6 \cdot 10^{-6}$ - $1.3 \cdot 10^{-2}$ Bq/m^3. The specific content of dust varied in range $3.2 \cdot 10^{-3}$ - $1.6 \cdot 10^{-1}$ mg/m^3.

Researches of collecting aerosols using filter compositions from fibrous materials was carried out to improve informational data and reliability of monitoring. This researches included.

1. Laboratory studies of filter properties of composite materials are fulfilled at increased linear air flow rate (80 and 160 cm/s), where, first layer (prefilter) was coarse-fiber FPP-70-0.3, PET-100-0.02 and FPS-110-0.2, second - thin-fiber FPP-15-1.5. By analysis results of experiments data was revealed possibility of qualitative estimation of aerosol dispersion and were obtained mathematical models of filter resistance growth due to dust accumulation, which helped to determine that composition FPS-110-0.2 and FPP-15-1.2 is optimal.

2. Real sampling of aerosols by two-layer filters was performed on a regular air sampling system of near ChNPP. The natural ^{7}Be, ^{210}Pb and ^{212}Pb were markers of submicron aerosols. Based on studies results carried out qualitative assessment of aerosol dispersion, which showed that radionuclides of Chernobyl's genesis of ^{137}Cs, ^{154}Eu, ^{241}Am were mainly on aerosols with AMAD more than 1 µm.

Analysis studies results showed that, firstly, aerosols distribution over the composite filter's layers depends on type of fibrous material of first layer and weather conditions during sampling of air. Secondly, prefilter assumes main dust load during intensive construction, erection works and earthworks. As FPP-15-1.5 filter is clogged more slowly with dust and that increased a lifetime of sampling system.

Using the filters composition in observing passage of radioactive cloud from the accident Fukushima-1 NPP in Ukraine from March 24 to May 16, 2011 allowed us to say that ^{134}Cs and ^{131}I were in air on submicron particles.

4CM.11

Reductions of PAH and Nitro-PAH Emissions from Diesel Engine by Using Micro-Emulsified Diesel-based Hydrous Glycerol Fuels.

SHENG-LUN LIN, Yen-Yi Lee, Fang-Ching Lee, Wen-Jhy Lee, *Cheng Shiu University, Taiwan*

Cleaner power generation technology is one of the way to deal with the major environmental problems, such as air pollution, human health, and global warming, coming with the uses of traditional fossil fuels. The major energy resources could be varied significantly depended on different country, and lead to several constraints on their greener energy development. For example, the electricity-powered vehicle could be a very “low emission” technique in the country that generate the power from “greener” processes (wind, solar, and hydraulic utilities). However, those techniques are technically hardly to be achieved in the country, who lacks those resources, such as Taiwan. Alternatively, the refuse-derived fuel became more important in a populated densely country. If the wastes of one manufacturer could be systematic transferred to energy resources of other producers, the manufacturing and waste treatment cost, pollutant and carbon emission, and health risk of the local residents might be effectively reduced by our local manufacturers. Therefore, the global economy impact to a local industry could be simultaneously reduced by this buffering system. This study focuses on the energy transformation techniques from wasted hydrous glycerol of the biofuel production processes to a diesel engine fuel. Glycerol was added into diesel by the fractions of 5–20 wt.% with the specific amount of surfactant additions. A homogenizer with 15,000 rpm was employed to emulsify the diesel blend by 5 min, and followed by an 750-kW ultrasonic homogenizer. A 90-day standing and the size distribution of glycerol droplets in diesel were done after the fuel preparation for ensuring they were well-mixed and thermodynamic stable. Furthermore, deionic water was added into pure glycerol by 20% to simulate the biodiesel-produced glycerol composition. Therefore, the stable blends, including G1, G5, G10, G15, and G20 (glyceral, G), were prepared as pure-glycerol-diesel fuels, while HG1, HG5, HG10, HG15, and HG20 (hydrous glycerol, HG) were hydrous glycerol-diesel blends. A 4-stroke, single-cylinder diesel engine generator (5 kW) with an output power control-measurement system, was employed to test the target fuels. The engine speed was controlled at “A” level, which is defined by European Stationary Cycle (ESC) as nlo + 0.25(n_{hi} - n_{lo}). Three loads, including 25, 50, and 75% of maximum engine load, were then tested. The emissions of PM, CO, and HC were monitored by a portable monitoring device (E8500, E Instrument.), while 16 PAHs and 6 *nitro*-PAHs were collected in particulate and gaseous phases separately by a stoichiometric sampling system. A GC/MS and a LC/MS-MS system were utilized to quantify PAHs and nitro-PAHs, respectively. Results shows that the brake specific fuel consumption (BSFC) were increase along with the increasing glycerol additions to the maximum 9.2%, while the heating value of G20 was 11.8% lower than that of pure diesel. The combustion enhancement of OH· provided by glycerol could partially balance the heating value effect. Additionally, the PM, CO, HC, particulate/gaseous PAHs, total PAHs, total BaP_{eq}, and total *nitro*-PAHs concentrations were all reduced significantly. These finding could also be resulted from that the oxygenated fuel have more fuel-containing O and was pyrolyzed to from more O· to easily initiate the combustion reaction. Also, lower volatility could also induce the low temperature combustion to prevent the soot formation. However, the NOx emission increased by glycerol addition, which is the major concern of the modern diesel engine. The better and more completely combustion of fuel provide higher heat release rate and temperature in the cylinder and increase the NOx level in the exhaust. Interestingly, the HG addition further reduce the NOx emission with, when the other pollutants were still inhibited. The optimal fuel based on pollutant emission concern is HG10, reporting an effective use of the waste biproduct from the biofuel production processes. Furthermore, the completely circular economically energy production could be achieved while the feedstocks (alcohol and fatty acid) of biofuel could be replace by refuse of waste material.

4CM.12

Preparation of Non-Woven PTFE Fibers Using Electrospinning. HAN-BIN KIM, Ki Bong Lee, Myong-Hwa Lee, *Korea Institute of Industrial Technology, Korea University*

Bag house system is commonly used to remove particulate matters in exhaust gases from various combustion facilities. Bag filter is the most important component to determine the performance of a bag house system. Bag filter made of PTFE polymer is widely used to collect particulate matters in dust-laden flue gas, due to its strong chemical resistance, low surface free energy. Especially, PTFE laminated membrane filter, which an expanded PTFE film is laminated on a woven glass fiber filter, is generally used in a bag house system because nonwoven PTFE bag filter is quite expensive. However, the filter has extremely low air permeability, which resulted in low filtration performance due to high pressure drop. PTFE foam coated filter, which has a high air permeability, was developed in our research group. However, the filtration efficiencies of the filter for fine particles are not high enough at initial stage of filtration, since the pore size of the filter is larger than 10 um1).

A new method was proposed to improve the performance of the PTFE foam coated filter in this study. The PTFE nanofibers fabricated by electrospinning were coated on a PTFE foam coated filter to decrease the pore size and improve the collection efficiencies for fine particles.

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Acknowledgment

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4CM.13

Investigation of Charge Decay Degree in Electret Filters with Various Surface Charge Densities. WOO JIN LEE, Jungho Hwang, Myong-Hwa Lee, *Korea Institute of Industrial Technology, Yonsei University*

PM2.5, i.e. particulate matters less than 2.5µm, is one of the major components that cause serious impact to a human respiratory system. Recently, many people utilize an air respirator and an air purifier to protect their body from fine particles. Electret filter, which is made by meltblowing a polypropylene polymer followed by corona charging, is generally used as a filter medium. However there are several reports that particle collection efficiency of the filter decreases over time by exposure to organic species and water(Motyl et al., 2006; Xiao et al., 2014). Many researchers tried to clarify the charge decay mechanism, however, it is still uncertain.

We investigated the charge decay degree in electret filters with various surface charge densities. As a result, we found that electret filter with higher surface charge density was more tolerable to isopropyl alcohol exposure than others.

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Acknowledgment

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4CM.14

Regeneration Characteristics of Filter Bag Cartridges with Various Pleating Geometries. JIN SIK KIM, Myong-Hwa Lee, *Korea Institute of Industrial Technology*

Pleated filter cartridge is a good alternative to treat a large amount of dust-laden gas in a limited space for a dust collector, because it has larger filtration area than a cylindrical filter bag. In general, the filter cleaning efficiency of a pleated filter bag is less than that of a cylindrical one and highly dependent upon pleat geometries, despite of its advantage. So far, the optimal pleating method of the filter media was not suggested yet. Dimensionless parameter, α, which is the ratio of pleat height to pleat width, is introduced to investigate the regeneration characteristics of a pleated filter cartridge in this study.

Six pleated filter bags with different pleat geometries (α=1.07, 1.36, 1.65, 1.93, 2.21, 2.50) and a cylindrical filter bag were prepared and tested in a lab-scale pulse-jet bag house system. The filter functioning antistatic water repellency was used as a filter medium and fly ash particles were introduced as the test particles. In addition, the filtration velocity was set to 1 m/min which is the usual filtration velocity in a real plant and the air flowrate maintained uniformly to have a constant filtration velocity by using a pitot tube and an inverter. Filter regeneration was conducted at the maximum allowable pressure drop of 100 mmH_2O under the clean-on-demand mode. The results showed that there was an optimum pleat geometry based on the filter cleaning characteristics of pleated filter cartridges, which had a maximum filtration area and reasonable filter cleaning efficiency.

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4CM.15

Conversion of Sulfur Dioxide and Nitrogen Oxides to Particulate Matter. MYONG-HWA LEE, Woo Jin Lee, Han-Bin Kim, Jin Sik Kim, *Korea Institute of Industrial Technology*

Sulfur dioxide, nitrogen oxides as well as particulate matters are coexisted in flue gas. Flue gas desulfurization for sulfur dioxide and selective catalytic reduction for nitrogen oxides, are usual control technologies. However, the equipment are too expensive to apply to a small-scale combustor. A new approach which converts them to particulate matter, was challenged in this study. The resultant species can be easily removed in a bag house system.
Sulfur dioxide concentration decreased drastically by injection of ammonia at the temperature of 200ºC. At the same time, drastic increase in particle number concentration was observed through the SMPS(Scanning Mobility Particle Sizer) measurement. However, there was no change in nitrogen monoxide concentration, even if the same amount of ammonia for SO_2 removal was injected in flue gas. Therefore, the effect of further oxidation of nitrogen monoxide to nitrogen dioxide on particle formation was also investigated. The characteristics of gas to particle conversion will be discussed in this study.

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4CM.16

Filtration Performance of Electret Filter Composed of Nano/Micron Fibers. TOSHIKI MURAKAMI, Takafumi Seto, Yoshio Otani, *Kanazawa University*

Air filters composed of electrostatically charged fibers (electret filters) are commonly used for respirators. In the present work, mixed nanofiber/microfiber electret filters were investigated in term of the filter quality factor. The mixed nano/microfiber electret filters were prepared by an electrospinning process. From the scanning electron micrographs of prepared filters, it was found that both nanofiber and microfiber were well mixed to form uniform packing structure. The average fiber diameter of nanofibers was 200 to 1200 nm depending on the spinning condition, while that of microfiber was controlled to be 1800 nm.

The filtration performance of filters was investigated by measuring the collection efficiency, E (=1-P, where P is the penetration) and the pressure drop. Test NaCl particles were generated by an evaporation-condensation method and they were classified by the differential mobility analyzer (DMA) into the monodispersed particles of 30 to 300 nm in the electrical mobility diameter. The number concentrations of DMA-classified aerosol at the inlet and outlet were measured by a condensation particle counter (CPC). The penetration through the electret was measured with and without electrical neutralization by soaking it with isopropanol. The filtration velocity was varied from 1 to 10 cm s^{-1}.

The filtration performance of charged and neutralized filters was evaluated by the filter quality factor, q_f, defined as the ratio of logarithm of particle penetration to the pressure drop: $q_f = -\ln P/\Delta P$, where, ΔP, is the pressure drop across the filter media. As the nanofiber diameter becomes smaller, q_f of charged filters increased and reached over 0.25 at the nanofiber diameter of 600 nm, however, q_f decreased when the fiber diameter was smaller than 600 nm. The total charge on the filter was estimated by comparing the collection efficiencies with/without neutralization. Q of the 600-nm fiber was estimated to be more than of 4×10^{-4} Cm^{-2} but it decreased with decreasing the fiber diameter.

Filtration performance of the electret was also analyzed by the single fiber filtration theory by taking into account the bimodal distribution of fibers. The filtration performance of the mixed fiber filter after neutralization was in good agreement with those predicted by introducing the inhomogeneous factor calculated from the bimodal distribution of fibers. As the fiber diameter decreases, q_f of neutralized filter increased as predicted.

4CM.17

Fine Particle Emission from Power Plants and Their Contribution to Air Quality in Korea. SUNGNAM CHUN, Suji Kang, Gayoung Lee, *Korea Electric Power Corporation Research Institute, Korea*

Now a day, the fine particle problem has become the most important air pollution issue in Korea. We occasionally experience the occurrence of high concentration events of particulate matter in the air that exceed the air quality standards during the spring season, and the Korean government is pushing various strict policies to reduce the emission of particulate matter. The goal of the Korean government is to low the fine particle concentration in the air by 30% in 2022 comparing with that of 2017. In Korea, the particulate matter is known to be contributed by the inflow of foreign countries and various domestic emission sources. Also it is considered that the contribution of power plants on fine particle concentration in Korea are approximately 4 % based on the 1st fine particles that are emitted as fine particles directly from stack and increase to 15 % including the second fine particles that are emitted as gaseous phase when these leave stack but converted to fine particles in the air through chemical reactions. Even though Korean government is trying to convert the energy portfolio from fossil to renewal energy era, until now more than 30 % of the electricity comes from fossil fuel sources, such as coal, oil and gas. Most of the fossil fuel used to make electricity is coal in Korea and demand of fine particle emission reduction is increasing.

This paper has summarized the assessment results of particulate emissions from Korean coal-burning power plant. We measured fine particle concentration in flue gas was measured using USEPA 201A and ISO 23210. We also measured the filterable particulate matter(FPM) and condensable particulate matter(FPM) and analyzed the chemical composition of particulate matter. The fraction of fine particulate matter to total particulate matter was assessed in coal-burning power plants. In addition, we reported the operating status of pollution control facilities, such as SCR, ESP, and FGD in a flue gas system from a boiler to a stack to assess the fine particle concentrations at each facilities and their fine particle removal efficiency.

To assess the contribution of power plants to the fine particulate matter concentration in the air, the background concentration monitoring station was constructed and we compared the concentration data obtained at the station with the measurement data obtained near the power plant. The fine particulate specimens which was collected at the back ground monitoring site and near the power plants were analyzed to assess chemical composition and we developed to assess the emission source apportionment.

In order to improve the air quality especially fine particulate matter concentration in Korea by reducing particulate matter emissions from various sources, it is necessary to identify the target sources and understand their emission characteristics. And it is also necessary to apply appropriate control technology to the emission sources. The data presented in this paper are considered to provide important information in establishing a control strategy for power plants as a large scale emission source to mitigate the fine particulate matter emission.

4DU.3

A Study on Pulverized Coal Combustion Using a Two-Stage Flat-Flame Burner with a Transition from a Reducing to Oxidizing Environment. Adewale Adeosun, DISHANT KHATRI, Zhiwei Yang, Richard Axelbaum, *Washington University in St. Louis*

Coal particles experience a transition from a reducing to oxidizing environment in the near-burner region of pulverized coal (pc) burners. For the first time, we report a fundamental study of ignition of a coal-particle stream experiencing a flame environment that transitions from a reducing to an oxidizing environment (termed reducing-to-oxidizing transition). High-speed videography is used to observe the particles in situ, and scanning electron microscopy is used to characterize the sampled particles. The effects of particle size on ignition are presented for four size bins (63-74 µm, 75-89 µm, 90-124 µm and 125-149 µm) for PRB subbituminous coal at two nominal gas temperatures (1300 K and 1800 K). The results show that the ignition modes under reducing-to-oxidizing conditions are different from those in purely oxidizing conditions, especially for small particles in a 1300 K gas temperature. The hetero-homogeneous ignition mode is dominant at the higher gas temperature, except for the 125-149 µm particle size range, where homogeneous-to-heterogeneous ignition occurs. For an 1800 K gas temperature, ignition delay time is relatively independent of particle size under either oxidizing or reducing-to-oxidizing conditions. However, the reducing-to-oxidizing transition increases ignition delay time by, on average, 100% over those of oxidizing conditions. At a gas temperature of 1300 K, ignition delay time depends strongly on particle size. For large particles (i.e., 90-124 µm and 125-149 µm), there exists a crossover at which the ignition delay times under reducing-to-oxidizing conditions are less than those under oxidizing conditions.

4DU.4

Nanostructure as a Paradigm for Describing Carbon Structure and Interpreting Its Formation. RANDY VANDER WAL, Madhu Singh, Joseph Abrahamson, Chethan Gaddam, Kuen Yehliu, Chung-Hsuan Huang, *Penn State University*

Combustion produced soot is highly variable with details as dependent upon Nanostructure – structure on the nanoscale has always existed. Yet recognition of its importance in governing carbon's chemical reactivity is comparatively recent. Nanostructure is generally described by the parameters of lamellae length, curvature (or tortuosity) and separation distance, measured perpendicular to the graphene segments. High resolution microscopy is necessary to access these scales with image analysis algorithms used to extract the spatial metrics. Aided by automated processing codes, distributions of each metric can be accumulated for their statistical description. Since 2004, nanostructure as a subject has appeared in more than two dozen papers. These studies have addressed nanostructure a) characterization, b) impact upon (carbon) oxidation, c) dependence upon molecular precursor and d) dependence upon combustion (i.e. formation) conditions, along with other related studies. Algorithms for nanostructure quantification provide measures by which to gauge the impact of these different formation conditions. Since the variations and more broadly formation conditions are generally specific to the source, nanostructure can serve as a paradigm by which to differentiate combustion sources by their combustion environments.

4DU.5

Towards Establishing a Semi-Empirical Soot Formation Model for Strained, Non-Premixed, Oxygen-Enriched Flames.

PHILLIP R. JOHNSON, Rajan K. Chakrabarty, Benjamin M. Kumfer, *Washington University in St. Louis*

The emission of carbonaceous soot particles to the atmosphere affects both the environment and human health. The presence of soot in industrial combustion systems also plays an important role for radiation heat transfer. For these reasons, prediction of soot fraction is often desirable in simulations of industrial boilers, furnaces and kilns using computational fluid dynamics (CFD). The complexity and size of these systems, in addition to limits on computational resources, often necessitates the use of reduced combustion models and simplified soot formation models. Many of the existing soot models are semi-empirical in nature and do not require large reaction mechanisms for fuel combustion because they are dependent only on the concentration of acetylene or the parent fuel. Existing models generally fall into two categories: one-step models in which total soot formation rate is calculated from a single Arrhenius expression, and two-step models in which nascent soot particle nucleation and surface growth are treated separately. However, most were developed for a specific application and/or validated under fuel-air combustion conditions only; their use in a different context, such as oxy-combustion, can lead to inaccurate predictions.

As reported in the literature, a soot-producing flame can become non-sooting (blue) with the combination of oxygen enrichment and fuel dilution, even while maintaining constant flame temperature. In addition, soot-producing flames may become blue with increasing strain rate. In this study, the accuracy of recognized and commonly used semi-empirical soot models is evaluated in response to oxygen enrichment and variable strain rate. The models are tested in a series of laminar counterflow flames which span the sooting-to-non-sooting transition. Flames are modeled using CHEMKIN with detailed fuel combustion chemistry. The gas-phase results are post-processed to calculate profiles of soot formation rate and volume fraction. Results indicate that existing models tend to overpredict soot formation in highly-strained flames and upon increasing oxygen enrichment, and do not adequately capture the sooting-to-non-sooting transition.

A new one-step semi-empirical soot formation model is proposed that aims to be applicable in a wide variety of flames. This model considers the effects due to changes in flame structure, caused by fuel dilution and oxygen enrichment, and also strain rate, on the soot formation rate. The model predictions are compared against experimental data from the literature for validation. Results demonstrate markedly improved accuracy for non-premixed, oxygen-enriched flames.

4DU.7

Submicron Ash Formation in Advanced Pressurized Combustion System.

DISHANT KHATRI, Zhiwei Wang, Akshay Gopan, Adewale Adeosun, Richard Axelbaum, *Washington University in St. Louis*

The novel Staged Pressurized Oxy-Combustion (SPOC) process, can reduce the efficiency penalty for carbon capture in coal-fired power plants by over half. The SPOC process incorporates a unique boiler configuration to enable combustion of pulverized coal at elevated pressure (15 bar) with low flue gas recycle. Although a promising technology for power generation, the impact on pollutants, such as the particulate matter (ash) has not yet been established. Therefore, in this work, the formation and evolution of sub-micron particles will be evaluated in a newly constructed 100-kWth pressurized oxy-combustor. The particle size distribution (PSD) of the sub-micron particles, and their morphology and composition will be measured using SMPS and SEM/EDX, respectively. Measurements will be carried out to study parametrically the factors which can affect submicron formation at the high pressure and high-temperature conditions. Parameters that can affect ash formation includes pressure, gas composition, and residence time. First, the effect of oxygen concentration (gas composition) at distance of 10 inches from burner tip, and 15 bar pressure will be studied to separate the effects of gas composition from those of residence time and pressure. To observe the effect of pressure, the pressure will be varied from 3 to 15 bar for a 30% oxygen concentration and at a distance of 10 inches from burner tip. Finally, to observe the effect of residence time, the particles will be sampled at 4 different axial locations keeping gas input composition at 30% oxygen molar concentration and a pressure of 15 bar. The experimental data, along with analytical models will help to understand the observed trends during these studies.

4DU.8

Employing Laser Pyrolysis to Generate Carbon Onion Particles and Its Application to Proton Exchange Membrane Fuel Cell.

JE HYEON YEON, Indae Choi, Sei Jin Park, Mansoo Choi, *Seoul National University, Seoul, Korea*

Various carbon nano-materials, such as graphene, carbon nanotubes and carbon black, have been used as supports for the catalyst particles in Proton exchange membrane fuel cells (PEMFCs) on account of conductivity and low cost. Due to the extremely high cost of widely employed pt catalyst particles in PEMFCs, it is desirable to load these particles on a robust support material such that the degradation of the support does not render the noble metal useless. Among the various forms of carbon, carbon nano-onions (CNOs) draw particular attention due to their concentric shells with high degree of graphitization. CNOs can be continuously synthesized by laser pyrolysis of hydrocarbon source (such as acetylyene and ethylene), and therefore has the advantage over other forms of carbon nano-materials due to the scalability of the production method[1].

Here, we present a CO2 laser induced pyrolysis of gaseous hydrocarbons to produce CNOs, and explore the parameter space toward the goal of producing CNOs over other carbon particles (such as amorphous soot). We demonstrate that the size, morphology and the number of graphitic shells are easily controlled by adjusting the experimental parameters. Owing to the high degree of graphitization, the CNOs show enhanced durability against oxidative potentials to commonly used commercial carbon materials such as Vulcan XC-72. Platinum-decorated CNOs have been used to fabricate PEMFCs and they are shown to have comparable performance to conventional cells, and the accelerated stress test reveals that the durability of the cells improved.

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4ED.1

Incorporating Engineering Context into General Chemistry Laboratory for a more Contextually Relevant and Engaging Experience for Engineering Students. CHANG YU WU, Kent Crippen, Lorelie Imperial, Corey Payne, Korolev Maria, Philip Brucat, *University of Florida*

The laboratory environment can offer valuable first-person, hands-on experiences that complement and extend the process of learning from other parts of a course. To this end, we are developing a unique laboratory curriculum for general chemistry for undergraduate engineers that more deeply engage students in authentic science and engineering practice. Our project involves a series of Design Challenges, which are problem-based laboratory activities based upon the NAE Grand Challenges for Engineering. These Design Challenges situate chemistry concepts and skills in an authentic engineering context with supports for the engineering design process. For engineering majors, contextualizing the learning of chemistry in such a way is theorized to strengthen the connection between the domain knowledge of chemistry and its application in everyday work, which enhances interest, efficacy, learning as well as retention. The user-centered design process enables us to keep our focus on the involvement of our target audience in all stages of development.

We will present our design framework, how results from usability testing are used to illustrate our iterative evidence-based development process. We will then present results of an initial pilot study from across one semester of student use (covering Grand Challenges topics of Restore and Improve Urban Infrastructure, Providing Universal Access to Clean Water, Making Solar Energy Economical, and Develop Carbon Sequestration Methods). For usability, data sources include video-recorded observations, field notes, student artifacts. For the pilot study, the assessed outcomes include chemistry content knowledge, self-efficacy, metacognition, and motivational variables. Both qualitative and quantitative analyses are used to address the research questions. The preliminary results showed positive changes in participant satisfaction, feeling like an engineer and for learning how to collaborate. Plans for additional re-design of the model and further study will be discussed.

4ED.2

NGDE: A Simple, MATLAB-based Code for Solving the General Dynamic Equation. JAMES CORSON, George Mulholland, Michael Zachariah, *University of Maryland*

The general dynamic equation governing aerosol particle nucleation, coagulation, and surface growth [1] is taught as part of undergraduate- and graduate-level college courses. This complicated integro-differential equation can only be solved analytically for a small number of special cases, so one must resort to numerical methods to solve the GDE. Unfortunately, the methods used to solve the equation often obscure the underlying physics: for example, moment methods (see e.g. [2]) transform the integro-differential equation into integrals that must be solved numerically for the various moments of the aerosol size distribution, while sectional methods [3-4] require assumptions about the size distribution within each bin. These considerations complicate efforts to understand the physics represented by the GDE.

To address these concerns, Prakash et al. [5] developed a code to solve the GDE using a nodal method, where aerosol particles exist only at discrete size nodes. This method is similar to the sectional method but obviates the need to consider intra-bin processes. Instead, the NGDE code uses a simple size-splitting algorithm – essentially, linear interpolation – to deal with particles that form or grow to sizes between two nodes. The original NGDE code was written in C; recently, we have converted the code to MATLAB. As part of the conversion, we have added several features to improve its function as a teaching tool, including implementation of a dynamic time-step algorithm that improves code stability and speeds up the calculation by orders of magnitude, and a post-processing tool that shows the evolution of the aerosol size distribution with time. We have also imbedded the Bohren Mie Code [6] in the post processing tool to show the evolution of the optical cross sections for the aerosol. Furthermore, because MATLAB is widely used in science and engineering curricula, users can more easily make changes to the code to add additional features or to implement different physics models for the constituent dynamic processes (e.g. substituting a different nucleation model in place of classical homogeneous nucleation theory with the self-consistent correction).

We will demonstrate the features of the NGDE code using sample problems including coagulation of an initially monodisperse aerosol, pure surface growth, and the full GDE for condensation of aluminum vapor. We will also discuss lessons-learned from including the NGDE code as part of an Aerosol Dynamics course at the University of Maryland.

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4ED.3

Aerosol Education with Community Citizens in Brandywine. AKUA ASA-AWUKU, *University of Maryland*

Here we describe an educational project launched with a community group in Brandywine Maryland (BTB Coalition), the University of Maryland, College Park and the AGU thriving earth Exchange to educate and inform local citizens of air quality and particulate matter concerns in the southern Maryland region. Successful community science requires skills and approaches that are not often emphasized or rewarded in traditional science research or education. This presentation will discuss the strategies, challenges, and outcomes to engage aerosol scientists with local communities in aerosol and air quality educational issues.

4ED.4

Image Analysis on Particle Size Distribution and Particle Tracking by Python-programming. CHIH-HSIANG CHIEN, Huanhuan Jiang, Wyndham Hudson, Bing Guo, Chang Yu Wu, Myoseon Jang, Paul Gader, *University of Florida*

The high-resolution camera has become popular and affordable in recent years. Image analysis from the camera can be processed by Python programming, which is not only reliable and efficient but also accessible for newcomers. In addition, Python has great libraries to support image analysis for free. Our laboratory has developed Python-based codes to analyze particle size distribution and to track particle motion on surface. We have applied the technique to an electrodynamic shield (EDS) system to understand the particle removal mechanism of EDS. Particle motion on soiling surface under a dynamic electric field was monitored by a microscope integrated with a digital high-speed camera. To determine the particle size distribution, each particle in an image was labeled and its area was determined by the number of pixels it covered. Frequency distribution was then calculated for size distribution. To obtain the particle trajectories, a three-step program was developed: 1) locate Gaussian-like blobs with a specified size in an image, 2) identify the same particle in different image frames, and 3) link the positions for a particle in each frame to generate a particle trajectory. The feasibility of these two programs was confirmed by inputting standard images with known particle size distribution and trajectories. The results showed the developed programs can successfully distinguish particles from images with varied geometry and generate particle trajectories. These two programs can serve as powerful tools for study of particle motion in air or on a surface.

4ED.5

Fundamentals of Air Pollution Engineering: A Free Online Resource for Aerosol Education. RICHARD FLAGAN, John Seinfeld, *California Institute of Technology*

The book Fundamentals of Air Pollution Engineering, 1988, is textbook that is available online in entirety for free. According to Amazon.com, it is "A rigorous and thorough analysis of the production of air pollutants and their control, this text for engineering students focuses on the formation and control of pollutants in combustion processes. The authors introduce the concept of air pollution engineering, providing an in-depth treatment of combustion, the formation of particulate matter and other pollutants, the principles of aerosol behavior, and basic theories of the removal of particulate and gaseous pollutants from effluent streams. In conclusion, they provide a framework for an optimal air pollution control plan. Suitable for advanced undergraduate and graduate courses in chemical, civil, environmental, and mechanical engineering, this volume assumes a basic familiarity with thermodynamics, fluid mechanics, and heat transfer. Supplements include new appendices, abundant worked-out examples and end-of-chapter problems, and a solutions manual, available from the authors upon request."

4ED.6

Combining Transferable Skills and Aerosol Science in Education. ANTTI LAURI, Taina Ruuskanen, Laura Riuttanen, Hanna Vehkamäki, *University of Helsinki*

We studied students' learning of transferable skills during a two-week research-intensive course. Advanced analysis of atmospheric aerosol and aerosol-related data was the topical emphasis on the course. The students were working on real data, and the project work they carried out during the course was a real research problem.

The transferable skills whose learning we studied were data analysis skills, academic writing skills, oral presentation skills, learning and teaching skills, and project and time management skills. All of these skills were included in the expected learning outcomes of the course. We invited the 30 students on the course to answer on a survey in the beginning of the course in order to find out about their expectations about learning transferable skills on the course. In the end of the course they answered on a second survey. The aim of the second survey was to find out how much they learnt during the course, and whether their learning on the course fulfilled their expectations.

The students on the course represented a rather mixed audience. Their stages varied between undergraduate students and postdoctoral researchers. The majority of the course participants were doctoral students. They also represented different disciplines: physics, meteorology, atmospheric science, Earth science, and biology.

We found that overall, the students felt they did learn the transferable skills included in the expected learning outcomes. The students found mixed groups in terms of stage of studies and discipline appreciated rather than problematic. Even more importantly, working with real data and research problems was considered motivating and rewarding.

4ED.7

Low-cost Particulate Matter Sensors: Developing, Piloting and Disseminating Appropriate Educational Resources to Support Community Use. Stefania Squizzato, Katrina Smith Korfmacher, Cait Fallone, Kathleen Gray, Dana Haine, John Prochaska, Diana Hernandez, Peggy Shephard, PHILIP K. HOPKE, *University of Rochester Medical Center*

A wide array of low-cost air quality sensors are available and have created opportunities for individuals and communities to monitor their exposure to a range of air pollutants (e.g., particulate matter, ozone). These sensors hold great promise for: enhancing environmental health literacy to promote behavior change that reduces exposure to air pollutants; enabling communities to investigate and document local sources of air pollution; and, supporting air quality focused citizen science and other environmental science education initiatives. However, users may not understand the resource requirements of various sensors, best practices for using the sensors to monitor their local environment, data uncertainties, and appropriate interpretation of results. This gap in knowledge may undermine effective use by individuals and communities. For example, users may mistakenly compare indoor air quality measurements and take action based on the recommendations outlined in the EPA's Air Quality Index (AQI) which only addresses outdoor air quality. Or users may overestimate the accuracy of sensor data, leading to frustration and mistrust when experts or agencies do not act on their findings. Better understanding of the potential and limitations of these sensors will help individuals and communities effectively use this new technology to better inform and promote actions that are protective of public health.

Low-cost air quality sensors have been used by citizen science, environmental justice and other non-governmental community groups to identify local sources of particulate matter and local patterns of ambient air pollution to inform public health action. Within the low-cost air quality sensor market, users are confronted with a range of sensors, each with different needs for and ability to access electricity, secure physical sites, Wi-Fi connectivity for downloading, etc. Similarly, in selecting a sensor, users may have different needs pertaining to pollutant(s) of interest, data accuracy, units, or reporting. Simply identifying the most accurate monitor, successfully capturing data, and providing platforms to share data with others does not adequately support community environmental health goals. Potential users need to understand the limitations of the technology (and resulting uncertainty) and the resource requirements of various sensors. They also need to know how to interpret their findings, especially in the context of the AQI.

The project presented here represents a collaboration between three National Institute of Environmental Health Sciences (NIEHS) Environmental Health Science Core Centers (University of Rochester, University of North Carolina-Chapel Hill and University of Texas Medical Branch) and their community partners (WEACT). The goal of the project presented here is to enhance users' understanding of air pollution and available sensor technologies in order to enable them to effectively choose, use and interpret sensor data in order to meaningfully address their community's public health concerns in three states (New York, North Carolina and Texas).

Specifically, this goal will be accomplished through (i) developing educational materials tailored to a community audience; (ii) evaluating the effectiveness of these educational materials by piloting them in four diverse communities and (iii) disseminating these materials through the NIEHS Partnerships for Environmental Public Health Network, along with other citizen science and environmental science education networks.

These educational materials will improve community stakeholders' capacity to select, deploy, understand and communicate the results of low-cost particulate matter monitors. By increasing community users' understanding of sensor technology, sources of uncertainty and how to interpret the results, our project will not only enhance the ability of communities to investigate and document local sources of air pollution but will also provide them with the resources to help them evaluate whether or not sensor use is appropriate in the context of their air quality concerns.

4ED.8

A Software to Map the Time-lapse History of Global Air Pollutions (TH-GAPs). MAOHUA PAN, Zechen Yu, Chang Yu Wu, Myoseon Jang, Paul Gader, *University of Florida*

Air pollutions, such as particulate matter (PM), NOx, Ozone, SO2, in heavily polluted areas can pose significant health effects to human beings. Time-lapse history of these air pollutants' concentration could help student better learn the global air quality patterns, while visualization of these data could also impress the public. Our lab has designed a software (TH-GAPs) to process data downloaded from Goddard Earth Sciences Data and Information Services Center (GES DISC) to generate a series of time-lapse videos for visualizing the dynamic behavior of global air pollutants. MatLab APP Designer is used to create the software. The observation or simulation data (e.g. ground level ozone concentration) are loaded into the software and then averaged according to the selected average time interval (e.g. 2 month) and/or the selected resolution (e.g. 1°x1°). Afterwards, these processed data could be saved and transferred to the second part of TH-GAPs to generate maps of the time-lapse concentration history of different air pollutants. Total ozone and ground level PM2.5 data from 2010-2016 were used to prove the feasibility of this software. Videos of the time-lapse ground level PM2.5 and total ozone concentration over South Pole, North Pole and around the world were successfully generated, and maps generated from this software are identical with maps from the National Aeronautics and Space Administration (NASA). Compared with commercially available software, the TH-GAPs is fast, convenient, open source and easy to share, and there are no strict requirements for the resolutions of the input data. This implies that Matlab App Designer can be used for software design to make air quality data processes faster and convenient, and to make air pollution results more illustrative and acceptable to the public. Our work demonstrates incorporating programming into environmental engineering can create better tools to engage people to care more about environmental problems.

4IA.1

Quantication of the Impact of Cooking Processes on Indoor and Outdoor, Primary and Secondary Organic Aerosols and Volatile Organic Species. IMAD EL HADDAD, Felix Klein, Andre S.H. Prévôt, Urs Baltensperger, *Paul Scherrer Institute*

Cooking is expected to be an important source of particulate pollution in indoor and outdoor environments. We conducted more than 100 individual experiments to characterize the particulate and non methane organic gas emissions from various cooking processes, their reaction rates and their secondary organic aerosol yields. We used these emission data to develop a box model, for simulating the cooking emission concentrations in a typical European home and the indoor gas-phase reactions leading to secondary organic aerosol production. We demonstrate that cooking dominates the particulate and gas phase air pollution in non-smoking European households. The gas-phase concentrations consist of about 60%, 20%, 10%, 9%, and 1% of small aldehydes, unsaturated aldehydes, larger aldehydes, acrolein, and terpenes, respectively. While frying processes are the main driver of the aldehyde emissions, terpenes are mostly emitted due to the use of condiments. Compared to primary aerosol emissions, which are dominated by frying processes, secondary aerosol production is negligible in indoor environments. In addition to providing an assessment of the impact of different cooking processes on indoor air, we will present a comprehensive framework for identifying the main parameters controlling indoor gas and particle phase concentrations. Based on the same emission data, we will also discuss the influence of cooking for outdoor air.

4IA.2

Three-Stage Modelling of Indoor Aerosol Formation Caused by Reaction of Ozone with Volatile Organic Compounds Emitted from Air Fresheners. Thai Phuong Vu, SEUNG-BOK LEE, Gwi-Nam Bae, *HoChiMinh University of Natural Resources and Environment*

A three-stage modelling of aerosol formation potential (AFP) was proposed to investigate secondary organic aerosols caused by ozone reaction of volatile organic compounds emitted from air fresheners. The AFP was defined as a function of formed aerosol mass per unit ozone reacted. The experimental system consisted of a reaction chamber, ozone and pure air generators and ozone and particle monitoring instruments. The volume of the cube-shaped reaction chamber made of 2-mil (about 51 µm) FEP Teflon film was 1 m^3 (1× 1× 1 m). The chamber was installed in a wooden box equipped with a door in order to avoid any light disturbances from the outside. The ozone concentration was monitored every one minute using a U.V. photometric O_3 analyzer (TEI 49i). The particle number size distribution was determined using a scanning mobility particle sizer (SMPS), which consisted of an electrostatic classifier (TSI 3081) and a condensation particle counter (CPC, TSI 3010). Total particle number concentration was also monitored using an ultrafine condensation particle counter (UCPC, TSI 3025) with a 1-sec response time. The air temperature and relative humidity in the Teflon chamber were maintained at 20^oC and 20%, respectively. The total sampling flow rate for monitoring particles and ozone in the chamber was controlled to be similar to the flow rate of ozone injected into the chamber. A 0.5-mL test specimen of a liquid-type air freshener was contained in a 50-mL glass petri dish with a diameter of 65 mm that was then placed in the bottom of the chamber. Ozone injection started after the test specimen was set and occurred into the center of the chamber through the top surface using a photometric O_3 calibrator (API 401). The ozone calibrator was operated at three different concentrations (50, 100 and 200 ppb) at a flow rate of 4.0 L/min. Each experiment lasted for 4 h. The aerosol formation process can be classified into three stages. The first stage of the AFP was determined at beginning time t_0 ($t_0 = 0$) to time t1 at which particle was not formed, $AFP_0 = 0$. The second stage of the AFP began from t1 to time t_2. There was a nucleation burst and conversion of formed particles to larger particles (size of 100 nm), $AFP_1 = a_1\Delta O_3 – b1$ ($a_1 = 0.4 – 1.9$ and $b_1 = 0.6 – 4.3$). The third stage of the AFP began from t2 to end experiment time t_3. There was stable increase in particle concentration, $AFP_2 = a_2\Delta O_3 – b_2$ ($a_1 = 0.7 – 3.0$ and $b_2 = 15.0 – 27.0$). Values of ai and bi were depended on concentration and quantity of biogenic volatile organic compounds in the air fresheners and ΔO_3 was ozone quantity reacted. The three-stage modeling was easy to be applied for investigation of the secondary organic aerosol formation under other environmental conditions such as ozone concentration, temperature, air freshener quantity, and initial volatile organic compounds. The three-stage modelling was easily and effectively used to evaluate and control secondary aerosol sources for indoor pollution management.

4IA.3

Impact of Household Daily Activities on Indoor Air Quality. Estela Vicente, Fernanda Oduber, Carlos Blanco-Alegre, Ana Isabel Calvo, Amaya Castro, Roberto Fraile, Teresa Nunes, CÉLIA ALVES, *University of Aveiro*

Household activities, such as cooking and cleaning, are known to generate considerable amounts of particulate matter indoors. In this study, the impact of four standard vacuum cleaners (washable filter bagless vacuum, wet vacuum, bag vacuum and a HEPA filter equipped robot) and two flat irons (steam iron and a steam iron with boiler) on indoor particulate matter levels was studied. The measurements were performed in León (Spain), in a house living room trying to reproduce the everyday conditions in late autumn (all the doors and windows were kept closed due to the cold weather outside - situation 1). Additionally, the particulate levels generated during steam ironing were also characterized while keeping the room doors opened and the windows closed (situation 2). On average, 45 min measurements were conducted during vacuum cleaning and 3 and half hours during ironing. After each household activity, the sampling continued until the restoration of particle concentration to the original level. Background indoor air measurements were also performed. A real-time laser photometric instrument (TSI, DustTrak DRX 8533) was used to record particulate matter concentration over time. Submicrometer particle number concentrations were measured using a Scanning Mobility Particle Sizer (SMPS, TSI Incorporated), which gives real time size distributions and number concentrations in the range from 7.64 to 310.6 nm. Simultaneous sampling with a PM_{10} high volume air MCV (model CAV-A/mb) instrument for gravimetric quantification was carried out. The equipment was operated at a flow of 30 m^3/h. Particulate samples were collected on pre-weighed 150 mm quartz fibre filters (Pallflex®) for gravimetric and chemical analyses. The gravimetric quantification was performed with a microbalance (XPE105 DeltaRange®, Mettler Toledo). After gravimetric determinations, thermo-optical analysis of PM_{10} filters was performed to obtain the carbonaceous content.

Regarding vacuum cleaning, the highest increase of PM_{10} concentrations and total particle number concentration was observed using the wet vacuum, 14.5 fold and more than 40-fold compared to background concentration, respectively. A 2-fold increase in PM_{10} mass over the background level was observed during the use of the HEPA filter equipped robot. $PM_{2.5}$ to PM_{10} ratios ranged from 0.43 (HEPA filter equipped robot) to 0.81 (wet vacuum). As regards the total number of particles, the readings were in the same order of magnitude, before, during and after the vacuum operation. Total carbon accounted from 9.0 ± 1.8 (wet vacuum) to 45.5 ± 4.1 (HEPA filter equipped robot) % wt. of the PM_{10} mass.

Average PM_{10} mass concentration in situation 1while steam ironing, without (191 ± 16 µg/m^3) and with boiler (180 ± 20 µg/m^3), increased more than 15 and 14 times compared to background concentration, respectively. Steam ironing under situation 2 conditions still increased the PM_{10} concentration 4.8 times (60 ± 17 µg/m^3). The lowest $PM_{2.5}/PM_{10}$ ratio (0.87) was observed during steam ironing under situation 2 conditions. Total particle number concentrations were from one to almost two orders of magnitude higher during ironing than prior to the start of the activity. Total carbon accounted for 30.4 ± 5.1 (steam ironing, situation 1), 51.8 ± 8.2 (steam ironing, situation 2) and 38.8 ± 3.1 (boiler steam ironing, situation 1) % wt. of the PM_{10} mass.

4IA.4

Reduction of Fine Particle Exposure for Bedrooms in Home According to Operating Conditions of an Air Purifier.

JUNHO JI, Gwang-Jae Lee, *EcoPictures Co., Ltd.*

Human indoor activities generate airborne fine particles which contribute to the increase of indoor fine particle concentration at home. Ultrafine particles are emitted during some activities e.g. burning candle or incense, cooking, spray use, computer printing and household cleaning (Gehin et al., 2008). Recently, interest in fine particles has been increasing in Korea. This makes it difficult to ventilate in house when fine particle concentration in outdoor air is high. Portable air purifiers are widely used at home. However, a portable air purifier at home does not seem to be used properly. The purpose of this study is to clarify the relationship between the reduction of particulate exposure and the operating condition of the air purifier, that is, the air flow rate. This gives very useful information for the consumer using portable air purifiers. At the same time, carbon dioxide was measured to propose a ventilation cycle in the family bedroom. We expect to reduce the public's anxiety against fine particles by supplying the field quantitative data. This study was conducted on the bedrooms of a small new apartment. The volume of each bedroom was 18.8, 22.8 and 24.84m3, respectively, and the test was conducted in an empty rooms. Area coverage of test air purifier was 29 square meter. An optical particle counter (OPC, portable aerosol spectrometer, model 1.109, Grimm, Germany) was used to monitor particle size distribution within the range 0.25–32 μm. An indoor air quality (IAQ) monitor (NDIR CO2 Detector, model IQ-610xtra, GrayWolf Sensing Solutions, USA) was used to measure the CO2 concentration in the range from 0 to 10,000 ppm. First, we measured the characteristics of natural decay of PM10, PM2.5, and PM1. The initial particle size distribution affected to the reduction of particle concentrations. The larger the particle, the greater the concentration decrease due to gravity. Continuous operation of an air purifier reduces indoor fine particles. Over time, relatively large particles were removed quickly and concentrations of PM10, PM2.5 and PM1.0 were similar. The results show that as the operation air flow rate of the air purifier decreases, the Clean Air Delivery Rate (CADR), which represents the performance of the air purifier, is lowered. Compared with the maximum airflow condition of the air purifier, CADR in the low air flow rate was reduced by about one third. Under the maximum air flow rate, the amount of fine particle exposure decreased to 10% when compared with the initial fine particle concentration and to 40% at the low air flow rate condition. When there was one person in a 24.84 cubic meter room, the carbon dioxide concentration increased to 1290 ppm for 30 minutes. The amount of fine particle exposure decreased to 20% and 60%, respectively for the operation conditions of maximum and low air flow rates. However, when there were two people in a room, the concentration of carbon dioxide in the room rose to 1250ppm for 30 minutes and 1970 ppm for an hour. In future research, we will propose the operating time of the air purifier considering the ventilation cycle which can effectively reduce the fine particle exposure in the indoor bedroom and the living room.

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4IA.5

Carbonaceous Particles and Gaseous Compounds in Kitchens and Outdoor Air of Different Homes. CÉLIA ALVES, Ana Rita Oliveira, Teresa Nunes, Estela Vicente, Susana Marta Almeida, Mário Cerqueira, *University of Aveiro*

We spend most of our time in indoor environments. As building infrastructures are increasingly air tight to save energy, epidemiologic studies need to understand the extent to which outdoor levels of air pollutants remain a determinant of exposure and, therefore, of health in the indoor environment. Many of the outdoor pollutants are also some of the most common contributors to unhealthy air inside homes, due in part to a ubiquitous and possibly surprising activity: cooking. Moreover, kitchens started to become living spaces and, in most cases, are the hubs of the home.

A monitoring program involving 4 kitchens with different characteristics and the respective outdoor air was conducted in the region of Aveiro, Portugal, in October and November 2017. Low volume samplers were used to collect particulate matter ($PM_{2.5}$) onto quartz filters, which were subsequently analyzed for their carbonaceous content (organic and elemental carbon, OC and EC) by a thermo-optical technique. Passive sampling of volatile organic compounds (VOCs) and carbonyls was also carried out.

Indoor and outdoor formaldehyde concentrations were 7.61±3.08 and 1.49±0.67 $\mu g/m^3$, respectively, whilst the corresponding acetaldehyde levels were 7.94±4.63 and 0.41±0.36 $\mu g/m^3$. Formaldehyde never exceeded the protection threshold of 100 $\mu g/m^3$ imposed by the Portuguese legislation. The mean indoor VOC levels ranged as follows ($\mu g/m^3$): benzene 0.92-2.9; ethylbenzene 0.80-1.7; toluene 3.9-9.3; m+p-xylene 2.4-5.8; o-xylene 1.0-2.2; styrene 0.27-1.5; 1,4-dichlorobenzene <0.10-1.2; trichloroethylene 0.35-2.5; tetrachloroethylene <0.10, and α-pinene 0.15-13.6. In general, all the kitchens except one registered indoor-to-outdoor VOC concentration ratios lower than one. The indoor levels of benzene, trichloroethylene, toluene, styrene and tetrachloroethylene were well below the thresholds laid down by the national regulations (5, 25, 250, 260 and 250 $\mu g/m^3$, respectively). Xylenes, toluene and styrene were highly correlated with each other, both indoors and outdoors, suggesting common emission sources.

The mean indoor $PM_{2.5}$ concentrations ranged from 13.8 $\mu g/m^3$, in the kitchen located in a rural area, to 30.2 $\mu g/m^3$ in a city center apartment with permanent occupancy. A mean outdoor level of 18.3 $\mu g/m^3$ was obtained in the rural area, while very close mean values were recorded in the center and outskirts of the city (27.6-29.5 $\mu g/m^3$). Total carbon (TC = OC + EC) accounted for about 30% of the $PM_{2.5}$ mass in the kitchens of the rural area and city center apartment. In the kitchens of houses with less central location, but near roads with intense traffic, the $TC/PM_{2.5}$ values were around 40%. The corresponding outdoor mass fractions ranged, in general, between 20 and 40%, the highest values being registered at the two locations more influenced by traffic. In general, the indoor OC/EC ratios were higher than the corresponding outdoor values. Regardless of location, ratios higher than 2 were usually observed. The highest OC/EC ratios were measured at the beginning of the sampling campaign, when the region was hit by wildfires.

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4IA.6

Aerosol Reduction Capability of an Air Purifier in the Real Living Room Environment. CHANG GYU WOO, Hak-Joon Kim, Yong-Jin Kim, Bangwoo Han, *Korea Institute of Machinery and Materials*

The concern to indoor air quality increased as people understand relation of air quality and health. According to a report, the market size will increase to $ 23.8 Billion by 2020. Many performance test methods including AHAM AC-1-2015 were developed, however, the performance test results are not directly translated to the environment of customers' houses. Air cleaning performance can be different because of air leakage, outdoor air quality, operation modes of air purifiers, and so on. An air purifier was deployed in a 36.8 m^2 living room of a house which is in Daejeon, Republic of Korea. Clean Air Delivery Rate (CADR) was calculated by varying experimental conditions with all doors were closed. KCl particles were used as test particles and were generated by using six-jet atomizer. The initial concentration of test particles in the living room was not critical to CADR values. Due to the air leakage of the house, outdoor $PM_{2.5}$ concentration showed negative relationship with CADR value. 10~30 $\mu g/m^3$ of $PM_{2.5}$ values were suggested as experimental range from the annual average of $PM_{2.5}$ concentration in major cities in Korea and from the CADR measurements in this work. This research can contribute to preparation of test method of air purifier in the real environment as well as understanding of air purifier operation in the real environment. This research was supported by National Strategic Project through the National Research Foundation of Korea (NRF) funded by Ministry of Science and ICT(NRF-2017M3D8A1091919).

4IA.7

Linking PM2.5 Indoor Air Quality and Emission Factors Measured during a Cookstove Intervention Trial in Rural India.

MOHAMMAD MAKSIMUL ISLAM, Roshan Wathore, Grishma Jain, Karthik Sethuraman, Hisham Zerriffi, Julian Marshall, Rob Bailis, Andrew Grieshop, *North Carolina State University*

Combustion of biomass in residential cookstoves is a major source of household air pollution (HAP), an acknowledged threat to human health. Although there are many studies showing the effect of biomass cookstove on HAP, there are limited number of studies where both emission and indoor air quality were measured across different seasons and at different locations. Thus, the quantitative linkage between cookstove emission and indoor air quality is still poorly constrained. In this study, we assess the effect of a cookstove intervention trial on indoor PM2.5 concentration as well as its seasonality and inter-site variability in two rural areas in India (Kullu in Himanchal Pradesh; Koppal in Karnataka). This study also aims to improve our ability to quantify the link between cookstove emissions and indoor PM2.5.

The study had three ~3-month-long measurement periods (baseline, follow-up-1, follow-up-2) for each location. Indoor PM2.5 concentrations were measured during ~5000 cooking events of traditional and alternate biomass and modern-fuel stoves. Measurements were conducted with real time mobile instruments (RTI micro-PEMS) which include a nephelometer and collect filter samples for gravimetric PM2.5 analysis. For a subset of those cooking events, simultaneous emission measurements were conducted by a portable instrument (STEMS). Kitchen performance tests (KPT) were performed to assess daily household fuel use. Use of stoves was measured using temperature-logging stove use monitors (SUMs) installed on all cooking appliances.

Preliminary data analysis for baseline showed that median indoor 24 hour average PM2.5 concentration in households in Kullu having Himansu Tandoor (improved chimney heating stove) as primary stove was 72 μg/m³, approximately a factor of two lower than for those with Traditional Tandoor stoves (142 μg/m³). A similar trend was observed during follow-up-1 (267 and 138 μg/m³ for Traditional and Himansu Tandoor respectively), indicating reduced pollution was associated with improved chimney stoves. Indoor PM2.5 for both stoves during follow-up-1 were twice as high as baseline, consistent with strong seasonality in PM2.5 concentrations. The households in Kullu and Koppal having LPG (either as primary or secondary stove) had median PM2.5 concentrations of 91 and 111 μg/m³ respectively, about 1.5-2 times less than households having no LPG stoves (142 and 207 μg/m³ in Kullu and Koppal respectively). The median PM2.5 concentration for houses having primarily traditional stoves was higher for Koppal (206 μg/m³) than Kullu (132 μg/m³), strong evidence of inter-site variability in PM2.5 concentration.

Stove-influenced (SI) periods were identified in the real time PM2.5 data using an algorithm and decay phase of SI periods were used to calculate air exchange rates (AER). Higher AER in Kullu households (11±5 h-1) compared to Koppal (7±4 h-1) may explain the reduced PM2.5 concentration in Kullu for the same stove. Average stove-influenced PM2.5 concentrations were higher during follow-up-1 (1127 and 1045 μg/m³ in Koppal and Kullu, respectively) than non-stove-influenced concentrations (45 and 26 μg/m³ in Koppal and Kullu, respectively). Moreover, stove-influenced PM2.5 concentrations were positively correlated (r2=0.89 & 0.79 for Koppal and r2=0.68 & 0.62 for Kullu during baseline and follow-up-1, respectively) with indoor daily average PM2.5 concentrations, indicating as expected, a strong association between cookstove emissions and indoor PM2.5. PM2.5 emission rate will be calculated using PM2.5 emission factor from emission measurement and fuel consumption rate from KPT. SUMs data will be used to identify cooking events associated with each stove types, and PM2.5 concentrations corresponding to those events will be obtained from SI analysis. Finally, with the help of AER and ventilation characteristics from household surveys, a statistical model will be developed linking emissions rate and indoor PM2.5 air quality.

4IA.8

Investigating Aerosol Emissions from Cooking Oils through a Controlled Chamber Experiment. , Sameer Patel, Itza Beltran, MARINA VANCE, *University of Colorado Boulder*

Cooking is an important contributor to aerosols in home environments. Cooking fumes, especially those produced by heating oils at high temperature can release a large amount of fine and ultrafine aerosols, which may lead to potential long-term hazards to human health. The objective of this study is perform a controlled chamber study to investigate the aerosol emission rates from a variety of popular cooking oils using an electric heat source at a range of smoke points: avocado oil, peanut oil, soybean oil, olive oil, coconut oil, and lard, both with and without the addition of salt, and at a variety of temperatures. Aerosol emissions are characterized in terms of size, volatility, and relative concentrations of black and brown carbon. Aerosol size distributions are characterized using a Scanning Mobility Particle Sizer (TSI) and an Aerodynamic Particle Sizer (TSI). The presence of black carbon and brown carbon will be investigated using an Aethlabs 5-wavelength aethalometer. Finally, aerosol volatility will be investigated using a custom-built thermodenuder. This study will aid in bringing indoor air quality field measurements into perspective by isolating cooking emissions from other potential indoor sources.

4IA.9

Particle Size Distribution of Indoor Aerosols, Natural and Artificial. HYAM KHALAF, Mostafa Mostafa, Mikhail Zhukovsky, *Ural Federal University*

Size distribution of inhalable aerosols is the most significant factor to predict aerosol deposition yield at various respiratory tract locations in human. Recently, electronic cigarette (EC), as the alternative of tobacco cigarette, is increasingly popular all over the world. However emissions from ECs may contribute to both indoor and outdoor air pollution and the number of users is increasing rapidly. In this investigation, mainstream aerosols generated from electronic cigarette were characterized in terms of particle number concentrations and size distributions by using diffusion aerosol spectrometer (DAS). DAS can be assessing in the range from 10-3 µm to 10 µm. Maximum number concentration of injected aerosol particles around 4x104 particles/cm3, most of these particle concentrations within the ultra fine particles (UFP) size range (0 to 0.2 µm) and the other in the size range from 0.3 to 1 µm. With time, the size mode of the particle number is less than 0.2 µm (UFP). The mass and the surface size distributions is presented and compared with bi-modal distribution.

4IA.11

Aerosol Release during Mechanical Solicitation of Tio2 Nano-Additived Paint. CHARLES MOTZKUS, François Gaie-Levrel, Nicolas Feltin, Stephane Delaby, *Scientific and Technical Center for Building (CSTB)*

The market of the nanocomposite materials in the construction industry is exponentially growing. Several types of nano-objects are currently used, in particular titanium dioxide (nano-TiO2). However, many questions are still open concerning the impact of these nanomaterials on the human health and the environment as previous studies showed. The degradations induced by the aging mechanisms could leads to the release of particles into the environment and today the chemical nature, size and concentrations are poorly known. In order to provide new scientific knowledge in this field, a research project called "EMANE" associating the CSTB and the LNE aims to characterize the particle release as a function of various aging scenarios for TiO2 nano-additived paints.

In this study, a nanomaterial called "model paint" was performed in laboratory, composed of an acrylic paint and 5% in mass of nanoparticle of nano-TiO2 (Aeroxide® TiO2 P25 Evonik Degussa). The physicochemical properties were characterized for this "model paint", and also for an acrylic paint and a commercial nano-additive photocatalytic paint. Samples of these three paints applied on the plasterboard plates (10x10 cm²) were submitted to different aging scenarios representative of environmental and use conditions encountered in indoor environments (humidity, temperature, oxidation, cleaning and mechanical solicitation).

The mechanical solicitations of samples were performed by abrasion by a TABER model 5750 linear Abraser. This device has a load arm which moves back-and-forth in a linear manner. The linear movement performed create a mechanical solicitation by friction at the tested material imply a particles released in the aerosol form. Test parameters such as stroke length, speed, load and the abrasive substrate used are adjustable. Two abrasion protocols have been developed. The first (stroke length = 7.6 cm, normal force = 8.3 N, velocity = 60 cycles/s, time = 30 s and cycles number = 30) corresponds to a strong abrasion removing the paint on the plasterboard plates and the second (stroke length = 7.6 cm, Normal force = 3.4 N, velocity= 75 cycles/s, time = 2 min and cycles number = 150) to a moderate with a partial abrasion of the paint. The abrasive substrate used (H18) is made of vitrified clay and has a diameter of 19 mm.

For each type of paint and scenario tested, three tests were carried out for each of the two abrasion protocols, corresponding a total of 165 experiments. In order to study the aerosol release associated with these two abrasion scenarios, the Taber abraser was installed in an experimental chamber to confine the aerosol and to move towards the aerosol emission to sampling isokinetic probes. The aerosols were characterized by real-time measurements (APS, DMS 500 and CNC3007) to measure the number concentration and the size distribution over a size range of 5 nm to 20 µm and by off-line measurements (MEB-EDX) carried out on aerosol samples.

The results obtained by DMS 500 and APS during abrasion on the "model paint" and on the commercial nano-additive paint samples show the emission of aerosols characterized by three particle populations around 60 nm, 200 nm and 2 µm. The results analysis shows the importance to normalize the number of particles emitted to the weight mass losses during an abrasion process for sample comparison. The study provide new scientific knowledge on the behavior of nanomaterials (TiO2 nano-additived paints) and especially on the aerosol released during mechanical solicitation. These new experimental data will allow us in the future to estimate the exposure of the people to manufactured nano-objects.

4IA.12

The Impacts of Cooking on Indoor Air Quality in Passive Houses. Ryan Militello-Hourigan, SHELLY MILLER, *University of Colorado Boulder*

Passive houses are a design concept to reduce energy use in buildings by making the structure tight and extremely insulated. This ongoing study is characterizing the indoor air quality of ten passive houses in Colorado by continuously sampling the air with optical particle counters while performing a repeatable prescribed cooking activity. Measurements are recorded while the occupants are away or minimally active for a period of approximately three hours. During this time, HEPA cleaners are also used to remove indoor ambient particulate matter. After the cleaning period, a hot plate is set up in the kitchen and one egg is fried in one tablespoon (15 ml) of canola oil. All buildings tested in this study feature either continuous or automatic ventilation systems with energy recovery and filtration. For each home, this cooking activity is performed while the homes' ventilation system operates at standard conditions, and then repeated several days later with the homes' ventilation system in "boost" mode for a period of 20-30 min. For the several days in between, a carbon dioxide monitor is also set up in the bedroom to measure daytime and nighttime concentrations. Preliminary results for fine particulate matter (PM2.5) indicate that outdoor particulate levels have little effect on indoor levels, likely due to filtered incoming air and low infiltration rates. PM2.5 levels quickly increase after cooking, but are slow to decay; concentrations generally stayed above the NAAQS 24-hour limit of 35 µg/m3 for over three hours for both ventilation modes. Using boost mode resulted in lower and higher concentrations for different homes, possibly due to variability in egg emissions. These early tests indicate that current ventilation practices may not be adequate for severe cooking events. Preliminary results for bedroom carbon dioxide levels show high variability across the homes with roughly half experiencing uncomfortable levels at night (> 1000 ppm). All ten passive house tests and analyses will be included in the final presentation.

4IA.13

Comparison of Physicochemical Properties and Toxicity of Particles Found Indoors and Outdoors in Occupied Residences – Measurement Methodology.

ANETA WIERZBICKA, Yuliya Omelekhina, Nicklas R. Jacobsen, Anne Thoustrup Saber, Erica Bloom, Patrik Nilsson, Axel C. Eriksson, Joakim Pagels, *Lund University*

Surprisingly little is known about toxicity and physicochemical characteristics of airborne particles found in residences, even though we spend about 65% of our time in homes. Characteristics and toxicity of outdoor particles have been studied and adverse health effects due to exposure have been confirmed. Outdoor particles infiltrate to indoor environments and we are exposed to them indoors but they change their physicochemical characteristics upon infiltration and mix and transform with particles and gas pollutants from indoor sources. Many indoor sources generate particles in amounts that exceed levels observed outdoors by far, for example during cooking or candle burning. There is a need to better understand exposures in homes. The aim of this study was to develop measurement methodology that would allow studying toxicity and physicochemical differences between particles found indoor and outdoor occupied residences.

Week-long measurements were conducted simultaneously indoors and outdoors in sixteen occupied residences in southern Sweden during winter time 2016/17. Residences included in the study were detached single family houses with natural ventilation and apartments with both natural and mechanical ventilation. Occupants kept logbooks of performed activities that were prone to generate particles.

Two identical sets of instruments for indoor and outdoor measurements were used. Instruments were placed in specifically designed enclosures to minimise the noise and disturbance for the occupants. Measurements comprised online assessment of physical characteristics of particles and collection of particles for off-line chemical analysis and toxicological studies in mice. Measured time-resolved physical characteristics were: number concentration and mean size (Nanotracer, 10-300 nm), $PM_{2.5}$ mass concentration (DustTrack DRX), and black carbon concentration (Microaethelometer). Filters from Dustracks DRX were used firstly for gravimetric analysis (corrections for DustTrack readings), then split into three parts and used for the following analysis: policyclic aromatic hydrocarbons quantification (GS-MS), metal analysis (ICP-MS) and ion chromatography. Particles were also collected on a Teflon filter for endotoxin analysis ($PM_{2.5}$ cyclone at flow 15 l/min). $PM_{2.5}$ particles for the toxicological studies were collected using Dekati Gravimetric Impactor (70 l/min).

Particles collected for toxicological studies were extracted and evaporated according to method described by Jalava et al 2005. In short each PTFE sample filter, was extracted twice in 30 ml methanol in ultrasonic water bath for 30 min below 35 degree C. All extracts of particles of one type namely: indoor, outdoor and blanks, were pooled together, sonicated and dried in a vacuum evaporator at 35deg C and 150 mbar.

During the measurement period we collected time-resolved data about physical characteristics of airborne particles indoor and outdoor occupied residences. Average particle number concentration (10-300 nm) was higher indoors than outdoors, and accounted to 6700 cm^{-3} (STD 4700 cm^{-3}) and 2400 cm^{-3} (STD 900 cm^{-3}), respectively. Gravimetrically assessed $PM_{2.5}$ mass concentration was higher outdoors than indoors, average outdoor concentrations were 8.5 μgm^{-3} (STD 6.1 μgm^{-3}) while indoors 4.9 μgm^{-3} (STD 3.7 μgm^{-3}). Extracted mass of particles collected for toxicological studies accounted in total to about 70 mg for indoor and outdoor separately, which was sufficient for conducting toxicological studies in mice, the results are being analysed. Preliminary tests of PAHs, endotoxin and metal analyses confirmed sufficient amounts of particle mass on split filters for the analysis, which are currently ongoing.

Applied measurement methodology proved its suitability for assessment of physicochemical characteristics and toxicity of particles found indoor and outdoor occupied residences. Collected and extracted $PM_{2.5}$ particle mass was also sufficient to perform toxicological studies in mice. These characteristics are needed to increase our understanding of the mixture of particles found indoors, in order to assess health effects and minimize exposure.

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4IA.14

Persistence of Wildfire-derived Pollutants in Indoor Environments. LUKAS KOHL, Meng Meng, Joan de Vera, Bridget Bergquist, Colin A. Cooke, Sarah Hustins, Brian Jackson, Arthur W. H. Chan, *University of Toronto*

The 2016 wildfire in Fort McMurray was the costliest disaster in Canadian history, forced the evacuation of all 88 000 residents, and destroyed 15 % of the town's the built structures. Re-entry was delayed after initial tests revealed elevated concentrations of organic and inorganic pollutants, including the toxic elements chromium (Cr), arsenic (As), and antimony (Sb). Currently, there are no studies that investigate how long wild-fire derived pollutants are retained in indoor environments, and if they represent a long-term health risk to residents.

Here, we report initial results from a house dust sampling campaign carried out 14 months after the fire. We collected house dust samples from the bedrooms of 35 houses using a modified vacuum cleaner. All analyses were conducted in the <150 µm size fraction. Trace elements were quantified by ICP/MS after total digestion with HNO3/H2O2/HF. We compare our house dust results with samples of urban and forest-floor ash collected during the Fort McMurray wildfire, background studies of Canadian houses in locations not affected by wildfires [Rasmussen et al., 2001, 2013], and regulatory guidelines (Alberta Tier 1 guideline for residential soils).

The concentrations of Cr, As, and Sb in house dust collected in Fort McMurray (geom. mean 48, 5.3, and 6.4 ppm) were comparable to those in background studies (geom. mean 101, 7.7, and 5.5 ppm [Rasmussen et al., 2001, 2013]. Ash concentrations of Cr, As, and Sb differed between urban and rural areas. Urban areas exhibited high concentrations (200-3000, 100-1300, and 20-300 ppm; n=3) that exceeded regulatory guidelines (64, 17, and 20 ppm), while concentrations in forest-floor ash samples were typically below those found in house dust samples (7-300, 1-12, and 0.1-3 ppm; n=5).

Overall, our results indicate that very high concentrations of Cr, As, and Sb can be found in ashes from urban, but not rural, areas; however, our data do not provide evidence that these elements persist in house dust over extended periods of time.

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4IA.15

In-field Emission Measurements of Forced-draft Pellet and Traditional Wood and Charcoal Stoves in Rwanda.

WYATT CHAMPION, Andrew Grieshop, *North Carolina State University*

Nearly three billion people rely on solid fuel burning stoves that emit particulate and gaseous pollutants causing adverse health and climate effects. In Rwanda, 96% of all homes utilize solid fuels for cooking, and wood is the primary cooking fuel in nearly all rural homes (GACC, 2012). Household air pollution (HAP) is the fourth highest risk factor for morbidity and mortality in Rwanda, and respiratory infection is the leading cause of life lost.

The current study assesses the Mimi Moto forced-draft pellet-fed semi-gasifier cookstove in urban and rural homes in Gisenyi, Rwanda. The objective of the study is to compare emissions of the Mimi Moto to traditional wood (three stove fire) and charcoal (coalpot/Jiko) stoves. The Mimi Moto is distributed through a unique business model that promotes availability and affordability, and provides the stove, delivery, training, and repair at no cost.

Uncontrolled cooking tests (UCTs) were conducted in 22 homes (2 tests per home) during November and December of 2017. A follow-up deployment of equal size is scheduled for May 2018, for a total UCT sample size of approximately 90. The UCT has the advantage over other test types (e.g., Water Boiling Test, Controlled Cooking Test) of being relatively unobtrusive and likely more representative of actual cooking practices. The Stove Emission Measurement System (STEMS) was deployed and measured real-time concentrations of carbon dioxide (CO_2), carbon monoxide (CO), $PM_{2.5}$ light scattering and absorption, and integrated filter $PM_{2.5}$ mass and organic/elemental carbon (OC/EC). Filter analyses are on-going, and additional analyses will include real-time emissions data (MCE, SSA), and particle optical properties (B_{ap}, B_{sp}) with a comparison against filter measurements. Field UCT results will be compared against field WBT results sampled using the same equipment.

Preliminary results found the Mimi Moto to have a 5- and 16-fold lower median CO emission factor (EF, g/kg) compared to the wood and charcoal stoves, respectively. Compared to previous field cookstove emissions studies (Roden et al., 2006; Grieshop et al., 2011; Wathore et al., 2017), median CO EFs were around 10-20% and 30% lower for wood and charcoal, consistent with inter-test variability for these traditional fuels. The Mimi Moto CO EF (20 g/kg) was higher than previously reported laboratory test results (conducted by a different group), highlighting the common observation that field tests may represent more realistic and “dirty” events compared to laboratory test results. The Mimi Moto stove also had on average 8- and 3-fold lower median test-average $PM_{2.5}$ light scattering compared to the wood and charcoal stoves. The distributions of Mimi Moto CO and $PM_{2.5}$ light scattering data were asymmetrical, clustered around a low mean value with a long upwards tail, suggesting that potential low emissions are not always realized in the field. This finding underscores the importance of proper stove usage. Properly functioning Mimi Moto stoves were clean-burning. However poorly operated Mimi Moto stoves were, for at least $PM_{2.5}$ light scattering, as dirty as their well-operated traditional counterparts. This study gives field evidence that forced-draft pellet-fed gasifier cookstoves have great potential to reduce emissions (and exposures), but may be highly sensitive to operational conditions.

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4IA.16

Exposure Assessment by Measuring Microbial DNA in House Dust using digital Polymerase Chain Reaction (dPCR).

ASHLEIGH BOPE, Samuel Cochran, David Kormos, Karen C. Dannemiller, *Ohio State University*

We spend 90% of our time indoors where we are exposed to diverse microbial communities. Much of this exposure results from house dust, which is resuspended from the floor due to occupant motion. This exposure may be assessed using quantitative Polymerase Chain Reaction (qPCR) using primers to specific microbial species of interest. Here, we explore the use of a new technology, digital Polymerase Chain Reaction (dPCR), as an advancement for measurement of this microbial DNA. Benefits of dPCR over qPCR include that it is less prone to inhibition and provides results in number of strands of DNA measured, potentially reducing the need for standards. To test measurement accuracy, we spiked known concentrations of *Aspergillus fumigatus*, *Escherichia coli* and *Bacillus atrophaeus* into carpet, vacuumed the dust, extracted DNA, and measured the quantity with dPCR. We determined that DNA was lost at each stage of the process, including vacuuming and DNA extraction. For instance, for *A. fumigatus*, 5% of DNA was lost in vacuuming from low pile carpet and 44% of DNA was lost in vacuuming from medium pile carpet. An additional 70% of DNA may be lost during DNA extraction. DNA extraction losses may be accounted for in qPCR through the use of appropriate standard, but could potentially be overlooked during dPCR. These results demonstrate the need to account for recovery efficiencies when using dPCR to measure microbial exposure from dust, or final results may be grossly underestimated.

4IA.17

Observed Levels of Particle and Gas Phase Pollutant inside School Classrooms with Varying Air-Conditioning Systems.

SUPREME JAIN, Divyam Garg, Anubha Goel, *Indian Institute of Technology Kanpur*

With the aim to examine air quality inside school micro-environments so that any possible health impact on students can be ascertained, a study was conducted inside two schools situated in the city of Kanpur, India which is one of the largest city (Inhabitants = 2.5 million) in the Indo-Gangetic plain. The two schools selected differed significantly in student strength, infrastructure, classroom size, ventilation system and proximity to the highways etc. Active air sampling inside classrooms was done continuously during the school timing (8:00 am to 2:00 pm) for particulate matter, and gaseous pollutants i.e. carbon monoxide (CO) and oxides of nitrogen (NOX).

In both schools, more than 99% of the sampling time PM10 mass concentration was higher than permissible limits (100 µg/m3 for ambient air) specified under National ambient air quality standards (NAAQS, India). The average PM10 mass concentration ranged between 200 to 240 µg/m3 during sampling hours (values ~ 2 times higher than permissible levels.) Type of ventilation system installed showed an impact on levels of respirable and finer particles with lesser levels observed in the school with a central cooling system. School which has air-conditioned classrooms were found to have PM3 concentration ~50% higher than permissible limits for PM2.5 (NAAQS, 60 µg/m3). The PM3 levels inside classrooms having a central cooling system were ~ 40% less than AC classrooms. Similarly in case of PM1 school having central cooling system had ~ 50% less mass concentration with respect to the AC classrooms. The average concentrations of gaseous pollutants (CO and NOx) were found to be within permissible limits during sampling hours. Influence of vehicular emissions in the vicinity of the school premises was observed through a sharp increment in finer particles and concentration of NOx inside the air-conditioned classroom during school opening and closing hours. Increased physical activity of the occupants inside classrooms was observed to raise the concentration of particulate matter but had less impact on the gaseous pollutants.

These observations highlight important role design of school building, and ventilation system, manmade or natural, installed play in affecting the indoor air quality. Chemical characterization of respirable particles is needed to enable realistic assessment of their impact on the health of the students. Diurnal variations in air quality in different microenvironments inside schools, such as playgrounds, library, canteen/ mess area, etc. need to be monitored and factors influencing levels and trends observed investigated. Lack of Indoor Air quality standards for different indoor micro-environments is another matter of concern and their development needs urgent attention.

Keywords: school, Indoor air quality, standards, particles, CO, NOx, ventilation, building design, air conditioning

4IM.2

Application of Particle and Aerosol Technology to CMP (Chemical Mechanical Planarization) Process Optimization.

TAESUNG KIM, Chulmin Shin, Seokjun Hong, *Sungkyunkwan University*

Chemical Mechanical Planarization (CMP) has become one of the most important and enabling semiconductor fabrication processes. Especially for logic devices, the number of CMP steps more than tripled from 28nm to 10/7nm node to enable complex integration schemes. However, there are still many aspects in CMP that have not been explained, which makes CMP rather art than science.

In this presentation, I will describe an effort to apply particle and aerosol technology to CMP process analysis to find a way to explain some of the phenomena more accurately. Firstly, Scanning Mobility Particle Sizer (SMPS), which is one of the standard instruments to measure particle size distribution, will be introduced for the measurement of slurry abrasive size distribution. Secondly, particle transport simulation with Computational Fluid Dynamics (CFD) will be introduced to predict pad debris transport between the wafer and pad, which can explain the pad debris trapping of laser drilled holes on the pad. Finally, new concept of pad debris removal to reduce scratch will be introduced.

4IM.3

Effect of O2/N2 Ratio on the Generation of Self-Charged Positive and Negative Sub 5 nm with a Glowing Wire. MICHEL ATTOUI, *LISA, Université Paris Est Créteil France*

Ultrafine particles generation with resistive heating wires (platinum, nickel, steel, tungsten etc…) in noble gases (argon, nitrogen, helium etc…) have been used since 1950s. Detection and sizing aerosol metrology (differential mobility analyzer coupled to atmospheric pressure mass spectrometers) highlighted the last decades that the lower limit in generated particles size of the method is around the atomic level.

The glowing wire method is mostly used with inert gases as carrier gases (nitrogen, helium or argon) to prevent contamination and especially oxidation.

Oxidation at high temperature on the other hand makes the wire very fragile and incapable to resist to a frequent breakages. However NiCr wire is the exception which is used in many industrial applications at high temperatures (ovens, heating, cooking etc…). This study focuses on the characterization of the glowing wire generator with a NiCr wire in a mixture of dry nitrogen-oxygen as carrier gas. The ratio of oxygen in nitrogen varies from 0 to 20 %.

The study is limited to sub 5 nm particles range in terms of size distribution of positive and negative self-charged particles with a high resolution DMA. The flowrate inside the glowing wire chamber varies from 10 to 50 lpm to prevent the growth of particles by coagulation.

4IM.4

Wide Size Range Number Concentration Calibration with Low Uncertainties. ANSSI JÄRVINEN, Jorma Keskinen, Jaakko Yli-Ojanperä, *Tampere University of Technology*

Aerosol instruments operate in a wide size range, which is a challenge in the instrument calibration. Different particle generation methods are used, and these require different concentration references. Instrument number concentration calibration in the small particle sizes, below 30 nm, is rather straightforward with different generation methods, bipolar charging and electrical classification with a Differential mobility analyser (DMA). Because at these sizes, particles acquire practically only one elementary charge, the Faraday-cup aerosol electrometer (FCAE) may be used as a reliable number concentration reference. The calibration size range can be extended towards larger particle sizes if multiply charging is minimized, but µm range is not typically achieved. The µm sized calibration particles are typically generated with completely different means. These methods do not produce singly charged particles, and as a result, different concentration references are used, for instance optical particle counters.

In traceable high accuracy calibrations, the step from the electrical reference to the optical reference is somewhat troublesome, because multiply charging limits the accuracy of the electrical method and the particle sizes below approximately 1 µm are problematic for optical particle counters as the detection efficiency may decrease. In addition, particle counters suffer from coincidence at high particles concentration, which limits the calibration concentration range. Thus, there is a need for a single calibration setup, which covers the size range from the smallest nm particles up to µm sizes.

To improve calibration accuracy in this problematic size range and to enable high concentration calibrations in µm size range, we have developed a calibration system relying on singly charged particles (Järvinen et al. 2018). The size range spans from nanometers up to micrometers, while the reference concentration is acquired from a FCAE. The developed system is an evolution of the Singly charged aerosol reference (SCAR, Yli-Ojanperä et al. 2010). The main principle is that singly charged seed particles are grown into larger sizes by condensing diethylhexyl sebacate (DEHS) on them. At large particle sizes, the process may also generate neutral particles, which must be removed with a DMA. To generate and classify µm sizes particles, a large sized DMA was designed and constructed. In a calibration measurement, large particles are divided between the instrument and the reference, which is sometimes challenging due to inertial losses. In our case, the concentration is equalized using a static mixer, which is followed by a flow splitter.

The operation of the calibration setup components was studied carefully. The particle growth was studied and DMA transfer function was measured. The major factors affecting the number concentration uncertainty were minimized and confirmed. The flow splitting was studied thoroughly with two identical FCAEs, and the bias between the inlet ports was observed to be small, less than ±1% from 3.6 nm up to 5.3 µm with uncertainty less than ±1% (k=2) at most of the size range at 1.5 l/min flow rate.

We used the developed setup in a calibration of a Condensation particle counter (CPC) detection efficiency. The detection efficiency was measured in the same size range with the bias, between 3.6 nm and 5.3 µm. The calibration uncertainty (k=2) was less than ±5% over the entire size range and less than ±2% between 5 nm and 4.3 µm.

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4IM.6

A Post-Correction Method to Improve the Accuracy of the Aerosol Particle Mass Analyzer. BO-XI LIAO, Chuen-Jinn Tsai, *National Chiao Tung University*

The available technique for the direct mass measurement of sub-50 nm nanoparticles is limited at the present time, restricting the characterization of the particle mass, density, and related properties. The tandem differential mobility analyzer (DMA) and aerosol particle mass analyzer (APM) provides an efficient mass measurement for submicron particles, while the lower limit of the particle size for the DMA-APM technique is restricted at about 50 nm due to the APM mass underestimation. To advance the technique for sub-50 nm nanoparticles, a post-correction method with an empirical equation according to the value of $\lambda_{c,P}$ was proposed to correct the APM mass underestimation without any modification of the instrument. The correction method was applied to the mass measurement data of the silver nanoparticles measured at different APM operation conditions. It was found that the standard error of the data fitting was reduced by the correction, suggesting that the quality of the measured mass data was improved by the correction. Besides, the study also confirmed that the influence of the particle size, porosity, and morphology of nanoparticles on the accuracy of the APM should be minor.

4IM.8

A Numerical Model To Predict The Performance Of High Flow DMAs To Classify Sub-nm Aerosols. HUANG ZHANG, Girish Sharma, Yang Wang, Shuiqing Li, Pratim Biswas, *Washington University in St Louis*

As conventional Differential Mobility Analyzers (DMA) such as Nano DMA do not have high resolution for classifying sub 2 nm particles[1], a Half Mini DMA was designed and fabricated to overcome these limitations[2]. In this presentation, a numerical computation was carried out to study the flow details inside the Half Mini DMA, and compare its classifying abilities for sub 2 nm particles with the Nano DMA. Because the flow rate designed in Half Mini DMA is high, a theoretical analysis is first performed to determine the flow compressibility under different working conditions. Second, the governing equations of sheath flow and electric field were developed. A transport-diffusion equation was used to describe the aerosol flow in considering the particles in DMA as continuous materials. Third, COMSOL was used to generate triangular meshes of the computational domain and solve all the governing equations. The results show that the velocity is much higher in Half Mini DMA than that of Nano DMA. Further, the transfer function of 1 nm, 1.5 nm, 1.8 nm and 2 nm particles were validated by the experiments, and to show that the Half Mini DMA does have a high resolution with sub 2 nm particles. Finally, the particle residence time and particle convective flux distribution were performed to explain the working ability difference of these two DMAs.

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4IM.9

Calibration of Centrifugal Particle Mass Analyzers (CPMAs) Using a DMA-Tandem-CPMA Technique. ZHEN LI, Jingkun Jiang, Da-Ren Chen, *Virginia Commonwealth University*

Instead of using the DMA-CPMA technique (i.e., a DMA is connected in series with a CPMA) often applied previous studies for the CPMA calibration, one DMA and two CPMAs were connected in series in this work to evaluate the performance of a CPMA (i.e., the particle penetration efficiency and the transfer function of a CPMA). This method is based on the operational principle of a CPMA, in which the centrifugal force acting on particles is balanced with the applied electrical force. The calibration of a CPMA should be directly based on the particle mass, not on the particle size classified by a DMA. In this DMA-tandem-CPMA experiment, particles of tested sizes were first selected by a TSI DMA. The mass-based size distribution of DMA-classified particles was then measured using the 1st CPMA. With the measured mass-based size distribution of DMA-classified particles, test particles of selected mass were classified by the 1st CMPA operated at fixed voltage and rotational speed. The test particle steam was then directed into the 2nd CPMA operated at the same rotational speed as that of the 1st CPMA while varying its voltage in an entire applicable voltage range. A condensation particle counter (CPC) was utilized to measure the concentration of particles exiting the 2nd CPMA. Polydispere solid particles of various materials were generated by spraying solutions of test materials via a custom-made Collison atomizer and drying generated droplets in a diffusional dryer.

We found that in the cases of particles with the mobility diameter larger than 100 nm, the particle mass measured by the 2nd CPMA was in general less than 10% of that classified by the 1st CPMA when test particles were selected from the right-hand side of mass-based particle size distributions. The particles mass measured by the 2nd CPMA agreed well with that classified by the 1st CPMA when they were selected from the left-hand side of the mass-based size distribution. In the cases of particles in the mobility diameters less than 100 nm, the particle mass measured by the 2nd CPMA were in general larger than 15% of that classified by the 1st CPMA when selected from the left-hand side of mass-based DMA-classified particle size distributions. Reasonable agreement between the classified and measured particle mass was observed when selected from the right-hand side of the mass-based particle size distributions.

Based on the measured particle penetration efficiency in the experiment, the transfer function of a CPMA were evaluated via a piece-wise linear inversion scheme with the assumption of the same CPMA transfer functions of both used CPMAs. The details of this work will be presented in the conference.

4IM.10

Characterization and Performance of the Caltech-ADI Portable Scanning Electrical Mobility Spectrometer. STAVROS AMANATIDIS, Huajun Mai, Changhyuk Kim, Richard Flagan, Steven Spielman, Gregory Lewis, Susanne Hering, *California Institute of Technology*

In this study, we present the detailed characterization and preliminary performance of the *Caltech-ADI Scanning Electrical Mobility Spectrometer (SEMS)*, a newly developed and highly portable particle sizer designed primarily for planned atmospheric studies.

The instrument combines a novel, compact radial-flow Differential Mobility Analyzer (DMA) developed at Caltech, and a self-sustaining, motion-tolerant, water-based condensation particle counter (WCPC) designed by Aerosol Dynamics Inc. The system operates at low flowrates (0.6 – 0.9 L/min, and 0.3 L/min for sheath and aerosol flows, respectively), and provides particle sizing in the 10-500 nm range with resolving power on the order of 2-3; this resolution and these flow rates are sufficient to attain the precision and counting statistics required for atmospheric measurements. The reductions from traditional operating parameters in SEMS measurements has enabled dramatic reductions in the volume, weight, pumping, and power requirements (<5kg, <50W).

The transfer function of the radial-DMA has been determined over the operating range of sheath/aerosol flows and voltage using highly monodisperse NaCl particles in the 10-500nm range. Moreover, we have explored the effect of voltage scan time to determine the extent to which the transfer function is smeared due to the delay time distributions in the plumbing and WCPC. This is especially important for Unmanned Aerial Vehicles (UAV) measurement applications where fast scans (<30s) are required to attain good spatial resolution of the atmospheric aerosol properties. The results are compared to theoretical transfer functions, as well as simulated ones calculated using COMSOL 3D finite element modelling. Further, based on the experimentally determined transfer functions, we compare the Caltech-ADI SEMS to a benchtop Scanning Mobility Particle Sizer (SMPS) in measuring ambient aerosol particle size distributions.

4IM.11

Mobile Chasing Measurement of Black Carbon and Nitrogen Oxides Emissions from Heavy-duty Vehicles in China.

SHAOJUN ZHANG, Hui Wang, Ye Wu, K. Max Zhang, *Cornell University*

The measurement techniques of vehicle emissions have achieved substantial advances in recent years, which have spurred the progressive implementations of stringent emission regulations. Notably, portable emissions measurement systems (PEMSs) have played an essential role in regulating real-world vehicle emissions. However, although the PEMS testing method has the useful features, the expensive instrumental cost and long experimental duration may become limitations to measure emission factors of massive on-road vehicles. Thus, we see a need for cost-effective and fast-response vehicle emission measurement methods to be developed and improved. In this study, we integrated a mobile measurement platform by equipping one Mini Van with multiple high-accuracy analyzers for measuring instantaneous concentrations of CO_2, CO, NO/NO_X, particle number, and black carbon (BC). For example, one EcoPhysics Analysator (Model CLD66) was applied to record continuous NO_X concentration profiles on the road, while one Aethalometer (Model AE-33) was used to measure real-time BC concentration. According to the concentration elevation ratios of targeted pollutants to CO_2 compared with road environmental baselines, fuel consumption-based emission factors of individual trucks are estimated. Comparative studies were conducted between PEMS and mobile chasing for BC and NO_X emission factors of typical diesel trucks, which provided sufficient evidences for the effective measurement of real-world emission factors using the mobile platform.

This mobile platform was further applied to measure emission factors of on-road diesel trucks on highways. During 2017 and 2018, we launched a large-scale field study in several provincial regions of China (e.g., Beijing, Tianjin, Hebei, Henan and Sichuan), in which nearly one thousand trucks were measured by chasing on typical highways. Our preliminary results show the China IV diesel trucks could effectively reduce BC emissions than the older China III trucks. Nature gas-powered trucks and buses emit significantly lower BC than the diesel engines by at least one order of magnitude. However, relative to China III diesel vehicles, we could find no significant improvements in NO_X emission factors for either China IV diesel trucks using selective catalytic reduction or nature gas fueled vehicles. These findings have highlighted great challenges to control NO_X emissions from modern heavy-duty fleets in China and will be useful to update road emission inventories.

4IM.12

A PPWD-SDEP-IC System for Hourly Measurements of Ambient PM2.5 Inorganic Ions and Precursor Gases. CHI-YU TIEN, Chao-Ting Hsu, Ssu-Yin Lai, Yung-Chen Chiang, Chuen-Jinn Tsai, *National Chiao Tung University*

A 2-stage Semi-Dry Electrostatic Precipitator (SDEP) was developed and integrated with the parallel plate wet denuder (PPWD) and IC as a PPWD-SDEP-IC system for hourly monitoring of $PM_{2.5}$ inorganic ions and precursor gases measurement. Carbon fiber bundles are used as the discharge electrodes in the first stage to lower the background concentrations of NH_4^+ and NO_3^- which are artifacts due to corona discharge of the traditional EP. The second stage of the SDEP is to collect charged particles in the electric field. The SDEP has the particle collection efficiency as high as 93-100 % for 14-700 nm NaCl particles generated in the laboratory at the operating flow rate of 5 L/min, and $PM_{2.5}$ collection efficiency of 98.1 % for incense smoke (MMAD of 241 nm). The inorganic ion recovery efficiencies of lab-generated non-volatile particles (Na_2SO_4, $(NH_4)_2SO_4$) and volatile particles (NH_4NO_3) are very good, which are 95% for Na^+ and 90% for SO_4^{2-}, 110 % for NH_4^+ and 90 % for SO_4^{2-}, as well as 107% for NH_4^+ and 99% for NO_3^-. By combining the $PM_{2.5}$ inlet, SDEP, PPWD, IC and automatic extraction and injection system, the PPWD-SDEP-IC system was demonstrated to have a very good performance for ambient $PM_{2.5}$ inorganic ions and precursor gases monitoring in the field comparison tests in which manual porous metal denuder sampler (PDS) and honeycomb denuder sampler (HDS) were used as references.

Keywords: PPWD-SDEP-IC, electrostatic precipitator, $PM_{2.5}$, aerosol sampling, inorganic soluble ions

4IM.13

Ultrahigh Resolution Orbitrap Elite Mass Spectrometry Reveals Unprecedented Molecular Detail in Atmospheric Aerosol. LYNN MAZZOLENI, Simeon Schum, Matthew Brege, Tyler Leverton, Elizabeth Rose, Maryam Khaksari, *Michigan Technological University*

Atmospheric organic aerosol is a very complex mixture containing components ranging from hydrophobic condensed aromatics to highly oxidized molecules. The compounds include C, H, N, O, and S, where N and S can exist in either oxidized or reduced forms. Ionization methods control what type of molecules are introduced into a mass spectrometer, thus a variety of ionization methods can be used for an accurate assessment of the overall organic aerosol composition. Specifically, the combination of electrospray ionization and atmospheric pressure photoionization is ideal for widespread coverage. Identification of unambiguous molecular formulas for accurate mass measurements requires low measurement error and sufficient mass resolution to separate common isobars. One of the commonly observed isobars in atmospheric aerosol involves molecular formulas that differ by 3.4 mDa due to the exact mass difference of C3 vs. SH4.

The ultrahigh resolving power of the second-generation high field Orbitrap Elite mass spectrometer (R = 240,000 at m/z 400) is sufficient for separation of common aerosol compositional isobars up to ~ 500 Da permitting an accurate assessment of S-containing compounds. The accurate mass measurements of the Orbitrap Elite can be further improved using a combination of custom internal and external calibration methods to refine the assignment of unambiguous molecular formulas. This is especially critical for compositions that include N and S, since the number of possible equivocal molecular formulas increases with increasing molecular weight. Thus, accurate mass measurements with less than 1 ppm mass error are needed to reduce the equivocal formulas.

In this presentation, we will demonstrate the power of ultrahigh resolution Orbitrap Elite mass spectrometry (MS) measurements with a focus on new ionization methods that provide new insights on the detailed molecular composition of ambient organic aerosol. We also present unprecedented molecular complexity using a segmented scanning approach with ultrahigh resolution MS/MS. These results suggest that a wide range of components from hydrophobic condensed aromatics to highly oxidized molecules are present in the aqueous extracts of organic aerosol. A more thorough understanding of organic aerosol composition is vital for an improved estimation of aerosol properties and studies involving fate and transport of pollutants.

4IM.14

Particle Measurement Under High Pressure Conditions on a Combustor Test Rig. Frank G. Bachman, TRISTAN REINISCH, Bill Silvis, Richard W. Frazee, Alexander Bergmann, *GE Aviation*

Until now, the only fundamental aerosol measurement approach available for an aviation turbine engine involves aerosol measurements taken at the exit plane of the aviation engine via fundamental particle measurement techniques. As the non-volatile aerosol measured at the exit plane of an aviation engine originates in, and is generated by, the combustor, it is highly desirable to be able to measure the aerosol at the exit plane of the combustor. The scientific drive, along with activities in the emissions legislation arena for aircraft engines, motivated us to investigate a particle measurement approach allowing for the measurement of the aerosol at the combustor exit plane.

We introduce a pressure reduction unit which is optimized for particle measurements applicable to the emission characteristics at the aviation turbine engine combustor exit plane. Particle loss mechanisms are considered and countermeasures reduce their influence. Particle Number Concentration, Particle Mass Concentration and Filter Smoke Number are the quantities used for characterization.

The pressure levels in a combustor of an aircraft turbine engine are much higher than those encountered in other typical combustion processes (e.g. internal combustion engines), where particle emissions are relevant and regulated. The commonly used measurement equipment is not designed to operate under such conditions. Thus, there is a need to reduce the pressure of a combustor exit plane aerosol sample to ambient conditions. A pressure reduction unit with critical flow elements was engineered and characterized on a combustor test rig at GE Aviation.

The pressure independent results for non-volatile particle matter were compared to a proprietary Filter Smoke Number based system, developed by GE Aviation, which is specifically designed to measure at sampling system pressure levels above ambient pressure. In this study, we prove that the pressure reduction unit for particle measurement equipment operating at ambient pressure conditions fulfills all our requirements. We also prove that further measurement results are reproducible and comparable throughout the typically encountered operating fuel-air-mass ratio range of the combustor. This gives the opportunity to use the results for further combustor development, specifically the ability to design the combustor to specific nvPM requirements. To show also that this instrument can be used to investigate the emitted soot particles with respect to morphology, we took samples for Raman spectroscopy. The results show highly graphitized carbon with sp^2 hybridization which is typical for soot particles produced under high pressure conditions.

4IM.15

Evaluation and Sampling Efficiency of the Wet Dust Sampler (WDS) - a Water-based Method for Road Dust Sampling.

JOACIM LUNDBERG, Göran Blomqvist, Mats Gustafsson, Sara Janhäll, Ida Järlskog, *VTI*

Emissions of PM is a well-known problem, with great impact on human health. One of the largest contributors is the road traffic. Due to stricter regulations for exhaust emissions, the relative importance of non-exhaust emissions is increasing. Abrasion wear of both pavements, tyres and brakes contribute to non-exhaust emissions. These particles are both directly emitted but also accumulated on the road surface as road dust load. This road dust is suspended through the road surface and tyre interaction as well as the turbulence introduced by the vehicle.

To allow for studies of the emission potential for road dust, the road dust load must be quantified. To quantify the total available dust load, a measurement device, the Wet Dust Sampler (WDS) [1] was developed. The WDS has since its development been used extensively for measurements in Sweden and has since then been updated. This updated version has also recently been exported to Norway and Finland.

The WDS basic principle of operation is to perform high pressure washing of a defined road surface area. This washing can be performed using regular water, or to allow for chemical analyses, distilled water. The sample is transferred into a storage container by the means of compressed air.

Studies of how the machine and the settings used impact on the cleaning and sampling efficiency include several tests of the performance of the newest version. Features tested have been e.g. the repeatability of flushed water, the repeatability of collected water, the cleaning efficiency and the retention of dust in the system.

One of the initial studies focused on the cleaning efficiency in which repeated sampling was performed in the same point. This was done for three different pavements of type Stone Mastic Asphalt (SMA) with maximum nominal aggregate size of 16, 8 and 6 mm. These pavements were selected based on common usage in Sweden (mainly larger sizes) due to their resistance against abrasion from studded tyres. This study was performed in a laboratory setting with laboratory manufactured slabs of pavement. The road surface texture was then filled with a well characterised dust of known source.

The initial, limited results show indications of a high cleaning efficiency, all having less than 10% retained material after the first sampling.

Further results regarding

References

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4IM.16

Investigating Effects of Ambient Gas on the Ionization of Compounds by Secondary Electrospray Ionization Using Ultrahigh Resolution Mass Spectrometry. JIAFA ZENG, Kai Wu, Rui Du, Yuling Zhang, Dandan Huang, Zhen Zhou, Xue Li, *Jinan University*

Secondary electrospray ionization (SESI) is a soft ionization technique, which occurs under ambient conditions; samples can be directly ionized without pre-treatment. A wide variety of organic compounds, such as fatty acids, aldehydes, ketones, alcohols and alkenes, have been successfully detected by using SESI mass spectrometry (SESI-MS) based methods. The ambient gas in the SESI source can affect the ionization efficiency of target compounds and interfering chemicals (e.g., plasticizers), which is closely related to the sensitivity of the method. In this study, volatile organic compound (VOC)-free dry-air and pure nitrogen gas (N_2, purity 99.999%) were selected as the ambient gases in the SESI source, and the effects of different ambient gases on the detection of typical exhaled VOCs (indole and acetone) in human breath and interfering compounds (dibutyl phthalate and polysiloxane) were systematically studied by using ultrahigh resolution mass spectrometry. The preliminary results indicate that the signal intensity of indole and acetone were enhanced at the presence of dry-air and N_2, and the enhancing effects were higher when N_2 was used. In contrast, the signal intensity of dibutyl phthalate and polysiloxane were greatly decreased, especially when N_2 was present in the source. Effects of dry-air on the detection of other exhaled endogenous compounds and interfering chemicals are still under investigation and the flow rate of the ambient gas delivered into the source is also tested in the present study. The study will provide helpful information on the optimization of SESI source and benefit a better understanding of SESI process, which is essential for improving method sensitivity.

4IM.17

Charge Distribution Characterization of an Indirect Ionization Soft X-ray Operated under Various Test Gas Environments. SIQIN HE, Derek Oberreit, *Kanomax FMT, Inc.*

Based on measuring mass (m) to charge (z) ratio of samples, mass spectrometry (MS) techniques have their analysis performance rely on reliable and steady ionization methods. The Chemical Ionization (CI) technique, as one of them, has been favorably used to study organic species in gaseous and particle phases because of its gentle ionization, reduced fragmentation, and flexible ion polarity selection during the ionization process. The operation of CIMS requires a bipolar ion source to generate positive or negative reagent ions, where the radioactive ion sources Am241 and Po210 have been commonly used in virtue of their simple operation and steady charge distribution, which meanwhile also limits the use of CIMS in field due to the safety regulations over radioactive sources. To facilitate the application of mass spectrometry analysis technique in field measurements, new ionizers have been developed based on soft x-ray ionization as an alternative source for such aerosol particle measurements that require bipolar charge conditioning, and its potential to be utilized in different operation environments is of great interest.

The ionization performance has been proven to be significantly influenced by the charging environment, e.g. the polarizability and properties of ionizing gas, the moisture level, and the chemical vapor content. In this study, the indirect ionization soft x-ray charge conditioner was evaluated by investigating its charge distribution when ionizing H2O or amine molecules in various test gases, including clean dry air (CDA), high-purity nitrogen (N2), high-purity carbon dioxide (CO2), and Argon (Ar). In addition, the transporting tubing material has also been reported to have an effect on charge conditioning performance, so a measurement comparing charge distribution of this soft x-ray charge conditioner with or without silicone tubing was also conducted and reported.

4IM.19

Performance Study of the HR-ELPI+ Instrument. Sampo Saari, ANSSI ARFFMAN, Juha Harra, Topi Rönkkö, Jorma Keskinen, *Tampere University of Technology*

Data inverting methods in aerosol measurement instruments have significant influence on the resolution and quality of the result. A new ELPI instrument, High Resolution ELPI+ (HR-ELPI+, Dekati Ltd.) uses a modern iterative inversion calculation method to improve particle size resolution and data analysis. In this study (Saari et al., 2018), the performance of the HR-ELPI+ is critically analyzed by simulations and experiments in the laboratory and field conditions, and the results are compared to the conventional inversion data analysis method (cut-point diameter concept) and common reference instruments (e.g. SMPS, EEPS).

Operating principle of the HR-ELPI+ is the same as ELPI+ operation added with the data inversion software. The data inversion calculation method is based on the kernel functions (Järvinen et al., 2014) and iterative calculation routine resulting in determination of particle size distribution with enhanced resolution. The inversion calculation runs in real-time and is simple to use and do not require any adjustments nor optimizations from the user of the instrument.

The simulation studies included the effects of two different sources of noise: 1) signal dependent noise by variation of concentration, 2) constant electric noise by electrometer. To find out the effect of the particle size, GMD of the simulated aerosol varied from 5 nm up to 9000 nm (GSD was fixed to 1.5). To study the effect of the GSD of the simulated aerosol, GSD values were tested between 1.01 and 2 (GMD was fixed to 100 nm). To investigate responses against multimode particle size distributions, a typical bi-modal (nucleation and soot modes) particle size distribution from a heavy-duty diesel truck engine and typical atmospheric aerosol modes (nucleation, soot, accumulation and coarse mode) were simulated and tested.

In the laboratory experiments, performance of the HR-ELPI+ was tested against dioctyl sebacate (DEHS) and NaCl aerosol generated using a nebulizer. Typical diesel exhaust aerosol from a passenger car on a dynamometer was tested in the field experiments. Experimental set-up consisted of parallel test aerosol measurements with the HR-ELPI+ and other reference instruments. The reference instruments were Engine Exhaust Particle Sizer 3090 (EEPS, TSI Inc.), two Scanning Mobility Particle Sizer Spectrometer: nanoSMPS (TSI Inc.) and longSMPS (TSI Inc.) and high-resolution low-pressure cascade impactor (HRLPI, Arffman et al., 2014).

Simulations showed that the HR-ELPI+ inversion performs accurately for lognormal unimodal and multimodal size distributions in the size range of 10 nm – 9 µm. Experimental results confirmed the simulated performance with laboratory test aerosols and field measurements. The results also indicated that the performance of the HR-ELPI+ may suffer if the raw currents have electrical noise more than 1%. However, the HR-ELPI+ clearly produces better resolution and quality with a low oscillation risk compared to the conventional cut-point diameter concept of ELPI. The HR-ELPI+ also generally showed very similar size distributions and concentrations compared to the EEPS and SMPS reference devices.

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4IM.20

A Shaker Fluidized-bed Atomizer (SFA) for Nanopowder Dispersion with Stable Aerosol Concentrations.

CHI-YU TIEN, Wen-Cheng Gong, Chuen-Jinn Tsai, *National Chiao Tung University*

This study aims to develop a nanopowder disperser to generate aerosols with stable concentrations in long period of time. The home-made nanopowder disperser, called shaker fluidized-bed atomizer (SFA), consists of a dry aerosol atomizer, a nanopowder fluidization chamber and air-flow distributor. At the nanopowder fluidization chamber, 1 g of tested powder is placed. The main function of the air-flow distributor is to make sure the bulk nanopowder is fluidized and aerosols are suspended in the chamber uniformly. The suspended particles are sucked into the atomizer at the top of the chamber and de-agglomerated by high velocity jet from the critical orifice. As a result well-dispersed fine particles are generated. The size and mass distributions of dispersed particles were analyzed using SMPS and NCTU micro-orifice cascade impactor (NMCI), respectively, and particle morphology was observed by the TEM.

The results showed that the multi-wall carbon nanotube (MWCNT) aerosols dispersed by the SFA was stable in number, mass and surface area concentrations during 8-hr period. Both the size and mass showed the bimodal distributions with the mode diameter 165 and 453 nm, and MMAD of 0.18 and 1.28 µm, respectively. The TEM images displayed that MWCNT particles collected on the lower stage impactor were well dispersed and showed single-fiber like structure. Different kinds of nanopowders will also be tested in the future for further accessing the performance of the SFA.

Keywords: Nanopowder disperser, SFA, MWCNT

4IM.21

Calibration of Condensation Particle Counters Against an Aerosol Electrometer Over a Wide Range of Sizes with Minimal Charge State Uncertainty. JONATHAN SYMONDS, *Cambustion*

The use of a Faraday Cup Aerosol Electrometer (FCAE) as a reference standard for Condensation Particle Counter (CPC) calibration is a long-established technique which has been recently codified as part of ISO27891:2015. Using a FCAE is attractive as it exhibits high detection efficiency, independence from particle material and morphology, and is clearly traceable to primary standards. However, its accuracy relies on the assumption that each particle entering the FCAE possesses just one elementary charge. Given a Differential Mobility Analyzer (DMA, referred to in the standard as a Differential Electrical Mobility Classifier, DEMC) is used to size select particles prior to the FCAE and CPC under test, it is possible for particles of the intended electrical mobility, but of larger size and with more than one elementary charge to pass through the DEMC. These will not only be counted by the FCAE as more than one particle, but by being larger, will bias the size dependent counting efficiency curve. The standard describes mitigating this by taking great care as to the size distribution of source aerosol used, or to measure or calculate the fractions of multiply-charged particles. The technique below follows the mitigation route.

The primary source is a nebulizer, here filled with dioctyl sebacate giving a peak size ~320 nm and σ_g=1.9. Between the aerosol source and the “charge conditioner” (neutralizer) is placed an Aerodynamic Aerosol Classifier (AAC, Tavakoli and Olfert, 2013). This selects monodisperse aerosol at high resolution by aerodynamic diameter rather than electrical mobility, and is thus not affected by particle charge. The AAC is set to the same equivalent aerodynamic diameter as the DEMC’s mobility diameter (converting using the known aerosol density). The DEMC is hence only fed with monodisperse aerosol at the desired mobility size, and populations of particles at sizes greater than desired corresponding to higher charge states are effectively eliminated. Although it is possible to use a second DEMC and neutralizer in this role, this would only attenuate the higher charge populations in proportion to the charging efficiency of the neutralizer, still leaving uncertainty.

Data is presented showing a TSI 3775 CPC compared with a TSI 3068B FCAE over a size range of 50 nm–1.8 µm, showing a mean detection efficiency of 98%. This upper size, beyond the normal range of the TSI 3801 DMA used, is achieved by dropping its sheath flow. This resulting reduced resolution of the DEMC does not matter as the size accuracy and resolution desired to generate an efficiency curve is achieved by the AAC: the DEMC is required only to remove the uncharged and multiply-charged particles.

The technique is automatable given a single aerosol source can be used over a wide range, as there is no requirement for a close relationship between raw aerosol size and that selected in the DEMC. A continuously variable rotating disc diluter was used to keep the raw aerosol concentration within the optimal band for both the CPC and the FCAE. Although the lower limit of the current AAC instrument is 25 nm, below this multiple charging is not significant.

ISO27891:2015 also provides for calibration of a CPC against a reference CPC. In this case, there is no requirement for the aerosol to be charged, and an AAC can replace the DEMC. This is potentially useful in field calibrations where regulation prevents the use of radioactive or X-ray sources, and is possible up to the AAC size limit of ~6 µm. The technique is used to show that for particles >3 µm, single particle counting in the 3775 CPC breaks down.

4IM.22

Study of HR-ELPI+ Data Inversion with Porous Collection Substrates. ANSSI ARFFMAN, Ari Ukkonen, Anssi Järvinen, Sampo Saari, Esa Luntta, Ville Niemelä, *Dekati Ltd., Kangasala, Finland*

In this study, the effect of porous collection substrates on the data inversion algorithm of the HR-ELPI+ (Dekati Ltd.) was explored. The operation and verification of the inversion algorithm has been described and evaluated earlier for smooth collection plates (Saari, 2018). The porous collection substrates have been used in impactors to avoid particle bounce and to increase the loading capacity (e.g. Reischl & John, 1978; Van Gulijk, 2003; Tsai, 1995). The probability of particle bounce decreases and the loading capacity increases especially when oil is added to the porous collection substrate. The oil creates a sticky surface preventing the particle bounce, and the porous surface structure provides micro reservoirs for the oil, thus, keeping the impaction surface sticky even after several layers of particles has formed on a top of the collection substrate. The porous collection substrate also reshapes the impactor collection efficiency curve compared to a smooth or a plain surface. The cut size shifts to smaller size, the collection efficiency curve is less steep, and the fine particle losses will increase (see, e.g., Marjamäki, 2004). The increased losses influence to the 'tail' of the collection efficiency curve and also introduce the so-called excess collection efficiency in the sub-cut point particle size range as described in detail by Huang et al. (2001).

As stated earlier, the porous collection substrates decrease the cut points and reduce steepness of collection efficiency curves. Thus, it is important to evaluate how these changes affects to operation of inversion algorithm and results obtained when smooth collection plates are replaced with porous ones. The performance of HR-ELPI+ inversion was studied by numerical simulations and experimentally in lab conditions. The measured cut-sizes, collection efficiency curves, and fine particle losses for porous substrates were used in both studies.

In simulations, first, the theoretical current response of the ELPI+ for a log-normal size distribution was calculated and then the HR-ELPI+ inversion was used to calculate backwards the initial input size distribution. The results were then compared to the initial size distribution. In the experimental tests, the test aerosol generated from DEHS oil was measured with the HR-ELPI+ equipped with sintered metal substrates and the results were compared to the measurement results of the HR-ELPI+ with the normal smooth collection plates.

The simulation results showed that in the size range of 20 to 1000 nm the difference in number concentration between the inverted and the input concentration was 6% in maximum. For size distributions with GSD 1.3 or larger, the differences were smallest and the maximum differences were observed for narrow size distributions. The experimental tests showed that the similar accuracy can be achieved also in practice for evaporation-condensation method generated DEHS aerosols. Overall, results showed that the HR-ELPI+ inversion can be successfully used to retrieve the high resolution input size distribution although the porous metal collection substrates change the collection efficiency curves of the ELPI+ impactor in large extent.

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4IM.23

Comparison of the TSI 1-nm and Standard Scanning Mobility Particle Sizers during the Lake Michigan Ozone Study.

MEGAN CHRISTIANSEN, Charles Stanier, Sherrie Elzey, Nathan Janechek, Nathan Bryngelson, Maynard Havlicek, Andrea Tiwari, *University of Iowa*

During the Lake Michigan Ozone Study 2017 (LMOS 2017), the aerosol size distribution was measured for a 1-month period at Zion, Illinois, a site on the Western shore of Lake Michigan. The purpose of the field study was to establish an observational database for improved understanding and model-measurement evaluation of regional and local ozone episodes. Aerosols were monitored as a source apportionment and monitoring site characterization tool, together with extensive meteorology, remote sensing, and in-situ gas-phase monitoring. The study ran from May 22 – June 22, 2017.

The study was used as an opportunity to compare the widely used and well-established "long DMA" configuration of TSI's Scanning Mobility Particle Sizer (SMPS™ with model 3081 DMA column paired with model 3785 CPC), against a newly developed commercially available model 3938E77 1-nm SMPS capable of 1-nm sizing. The 1-nm SMPS combines a model 3086 1-nm DMA, model 3777 Nano Enhancer with diethylene glycol working fluid, and model 3772 CPC with butanol working fluid. The 3777 Nano Enhancer uses diethylene glycol to pre-grow particles to ~ 100 nm for CPC detection.

During a majority of the sampling campaign, the 1-nm SMPS was well correlated with the standard SMPS in the overlapping size range of 12 to 32 nm. Preliminary data analysis indicates that within the overlapping range, the mean particle concentrations were 1956 cm^{-3} (1-nm SMPS), 1272 cm^{-3} (standard SMPS), with a correlation coefficient (r) of 0.93. The correlation coefficient is calculated based on paired hourly data pairs (n=537). Counts were significantly higher on the 1-nm SMPS at sizes less than 20 nm, with increasing divergence between the instruments as size decreased. This is in part due to differences in inlet flows and particle losses between the two instruments.

Several nucleation and growth events were detected with this 1-nm SMPS configuration, with particles detected down to 1.2 nm geometric mean diameter. These events will be placed in context with the 3D and 2D wind fields measured at the site (by SODAR and anemometer, respectively), as well as high time resolution radiation and gas-phase measurements (VOCs, NOx, SO2, nitric acid). The percentage of hours with number concentrations greater than 50 cm^{-3} using the 1-nm SMPS in the 1 to 3, and 5 to 10 nm size ranges, was 28% and 73%, respectively.

Ongoing data analysis will further explore the above, as well as any differences in the size distribution caused by drying the standard SMPS while leaving the 1-nm SMPS undried. Finally, periods of very high, and seemingly non-physical, counts detected by the 1 nm SMPS will be explored.

4IM.24

Effect of Eccentricity on the Performance of a Cylindrical Differential Mobility Classifier. THAMIR ALSHARIFI, Da-Ren Chen, *Virginia Commonwealth University*

Scanning/differential mobility particle sizers are now commonly used in aerosol community to characterize the size distribution of submicrometer particles in gases. A differential mobility classifier (DMC) is the key component in the sizers for sizing particles. In the DMC design, it is required to provide the tolerance at least on all the key dimensions of a DMC when the mechanical drawing is produced for machine shops. The tolerance requirement in a DMC design also affects how the DMC is constructed. It is therefore very important to understand the design/construction imperfection on the performance of a DMC. Differential mobility classifiers in various configurations have been designed and evaluated in the literatures. Among different configurations, DMCs in the cylindrical design is the most popular ones because of no side-wall effect encountered in parallel-plate DMCs and their successfully commercialization. As the first step in a series of investigation, this study focused on the effect of eccentricity on the performance of a cylindrical DMC. Numerical approach was taken in this study. COMSOL was applied in the numerical modelling.

In this study, we investigated the effect of eccentricity on the performance of different cylindrical DMCs operated at different aerosol and sheath flow rates. The geometrical parameters of studied DMCs include the diameters of inner and outer cylinders, the length of particle classification zone, and the angles of aerosol entrance and exit. Prior to the parametric study, our modelling result was validated by the comparison with the theoretical transfer function given by Knutson & Whitby (1975). The theoretical transfer function derived by (Knutson, 1972) for an eccentric DMC in the cylindrical design was also included in the comparison.

Our study shows that, because of the eccentricity, the DMC transfer function was deteriorated as the eccentricity increased for Nano-DMA. The peak of DMC transfer function would split into two peaks as the eccentricity (defined as the off-center distance to the annular spacing between two cylinders) is more than 5%. This two-peak appearance of the transfer function would occur at the less eccentricity as the classification length of DMCs. However, the effect of eccentricity would be reduced as the annular spacing between outer and the inner cylinders was increased. More details of our study will be presented at the conference.

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4IM.25

Effect of Change in Sheath Air Humidity on Size Distribution Measurements by Scanning Mobility Particle Sizer. B.K. SAPRA, Mariam , Manish Joshi, Arshad Khan, *Bhabha Atomic Research Centre, Mumbai*

Scanning mobility particle sizer (SMPS) is widely used for measurement of size distribution of sub-micrometer particles in atmospheric and laboratory applications. Sheath air flow inside Differential mobility analyser of SMPS provides laminarity for aerosol particle stream flow. This work investigates the effect of sheath air dryer in the measurement of size distribution of particles with varying hygroscopicities. Aerosol particles of three different materials i.e. NaCl, $NaNO_3$ and nichrome generated by nebulization/electrical heating were sampled through a twin SMPS system from a controlled chamber of volume 40 L. As the particles (of NaCl, $NaNO_3$) generated from nebulization showed geometric mean diameter between 100-150 nm, nichrome nanoparticles were also allowed to grow in the same size range. One of the SMPSs of twin SMPS set-up had modified sheath air path (by keeping dryer in circuit) while the other was kept as such in a T-joint arrangement taking simultaneous sample from the chamber. Three sets of experiments were performed for each type of particle system at 3 different (chamber) relative humidity (RH) levels (15%, 40% and 90%). For the case of NaCl particles, 52.2±0.48% decrease in relative geometric mean (GM) of distribution measured by SMPS with sheath air dryer was seen at 90% RH. No such difference was noted for other RH levels (lesser than Deliquescence RH: 75.3% (Pilinis and Pandis, 1995). $NaNO_3$ particles did not follow any deliquescent behaviour (Hu et. al., 2010, Lee et al., 2011), and showed growth at lower RH (40%, 60%) levels as well. Size distribution of Nichrome metal particles measured by both SMPSs remained unperturbed at all RH levels. Experimentally measured changes in GM diameter for the case of nebulized particles were also found to be reasonably matching with KÖhler theory predicted values. Since there is no clarity on protocols for usage of sheath air dryer for SMPS measurements; correction factors, algorithm modifications, newer protocols are required to be incorporated for size distribution measurements.

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4IM.26

SEMS Transfer Functions under Fast Sequential Scanning. MARK KANAPARTHI, Suresh Dhaniyala, *Clarkson University*

The size distribution measurements are routinely made using a Scanning Electrical Mobility Spectrometer (SEMS). These measurements are generally made over a reasonably long time period (large scan time). With decrease in the scan time of the operation, the discrepancy between the classically predicted transfer function and the actual transfer function is more pronounced. As the scan time approaches the average residence time of the particle in the classifier section, an increasing fraction of particles that are injected during the scan are extracted in the successive scan. To calculate the transfer function under such conditions, the traditional trajectory approach by Dubey and Dhaniyala (2008) can't be employed since the particles encounter a combination of an exponentially increasing voltage with an exponentially decreasing voltage, i.e. the Arrival time Transfer Function (ATF) can't be translated in time as was done previously. The ATF's have be calculated for every mobility to compute the mobility transfer function. The mobility transfer function computed is used to calculate the instrument response. The implications of inverting data under a combination of up-scan and down-scan is discussed.

4IM.27

Performance of Fundamental Functional Feature on DMA (2). CHIRYO TSUNODA, *FES*

In the previous presentation, we have known that the performance of functional feature on DMA have given two typical important data. The linear data have already explained, hereinafter, we would like to explain with the non-linear data for the performance of the new response function of DMA.

Encouraged by the successful theoretical and mathematical description for the performance of the response function of DMA, we will explain the correction methods for the effect of diffusion loses and the broadening effect in the devices, and we will explain the evaluation methods of the PSL standard particles.

4IM.28

Performance of Fundamental Functional Feature on DMA (1). CHIRYO TSUNODA, *FES*

Ever since the publication of the analysis methods by Knutson and whitby (1975), differential mobility analyzer (DMA) has become most useful instrument for the research of aerosol science. However, over the past forty years, researchers in this community have not found out an accurate methods for the data analysis of DMA. To solve this longstanding issue, we have addressed the mathematical theory of the electrical mobility classification. Finally we come up with the new accurate response function which is called critically transferred response function (CTR function), if you will. CTR function are integral function and are composed by two transfer function and one distribution function of measuring objects. CTR function of DMA create two typical output data, one is linear data and the other is non-linear data. These output data are strongly related the distribution of measuring object.

Encouraged by these successful theoretical and mathematical treatment, we will explain the performances for linear output data in this first presentation. And, we will explain the typical performance for non-linear output data in the second presentation.

4IM.29

A Compact, Battery-Operable, Dual-Channel, Water-Based Condensation Particle Counter. SUSANNE HERING, Gregory Lewis, David Workman, *Aerosol Dynamics Inc.*

A compact, dual-channel, water-based condensation particle counter is being developed to provide simultaneous measurements of ultrafine particle concentrations in two separate flow streams. The reported parameters are the airborne number concentration of ultrafine and fine particles in each channel of the system. The size range of detected particles extends from 7 nm to several micrometers in diameter. The time resolution is 1 second. Envisioned applications encompass those requiring simultaneous measurements in multiple size fractions, or in two distinct physical spaces. The long term goal is a battery powered instrument that is wearable.

As with other condensation particle counters, this system relies on condensational enlargement to grow ultrafine particles to optically detectable sizes. Yet in contrast to those now available, the instrument being developed here provides the following advantages: (1) it uses water, rather than alcohol, for the condensational enlargement; (2) it can be operated in any orientation; (3) it tolerates tipping and jostling; (4) it detects particles as small as 7 nm in diameter and (5) it is compact.

The approach is a self-sustaining water-based condensational growth system commonly referred to as “MAGIC” (moderated aerosol growth with internal water cycling). The MAGIC technology captures water vapor internally, allowing sustained operation without need of on-board reservoirs. The growth tube of the MAGIC system has a continuous water-wetted wick that spans three temperature regions, the middle one of which is warmer than the other two. Water evaporation from the warmed, middle section provides the water vapor that creates the supersaturation for particle activation and growth. The cooler, downstream section captures this water vapor, while maintaining supersaturated conditions needed for droplet growth. Capillary action transports the water captured by this stage, and by the initial stage, back to the warmed mid-section, providing sustained operation. MAGIC has no liquid reservoirs, and thus is insensitive to orientation and motion.

For the dual-channel device presented here, two identical MAGIC growth tube channels are used, both operated at a sample air flow of 100cm^3/min. A common set of temperature controls ensures that the respective stages of each channel are operated at the same temperatures. Each growth channel is coupled to an independent optical detector which detects individual droplets to enumerate the number of concentration of condensationally enlarged particles. The optical detectors are newly developed and miniaturized to provide a compact system. The dual-channel growth tube and optics, excluding electronics and supporting components, measures approximately 6cm x 10cm x 10cm.

Laboratory evaluations have been conducted under a variety of temperature and relative humidity conditions. Testing with monodispersed aerosols has demonstrated a lower particle size limit of detection of 7nm for both sucrose and sulfate aerosols. The response is linear to the highest concentrations tested of 8x10^4/cm^3. For sampling ambient air, the standard deviation between the two channels was 2%.

4IM.30

Selective Collection in Particle Harvesting. MENG-DAWN CHENG, *Oak Ridge National Laboratory*

Application of magnetic collection has a long history to atmospheric source identification[1],[2],[3],[4],[5] and as the marker for indoor air pollution[6]. In fact, most elements in the periodic table and their oxide forms are paramagnetic. Thus, magnetic collection could provide an effective means of environmental sampling of aerosol particles that consist of magnetic materials. This would in essence enhance the analyte signal by selectively collect particles consisting of only relevant composition at the time of collection. To trigger selective magnetic material harvesting from airborne particulate matter, first the magnetic circuit needs to generate high-gradient magnetic field density on the order of a few Tesla (T) per meter. The recent advance in additive manufacturing of permanent magnets enable the design of such a circuit with the magnetic field density around 16 T/m, which makes selective collection of aerosol particles by their magnetic property in a small footprint and with a low-power consumption mode possible.

In this presentation, we will report the development of a particle selective collector based on a HGPMS circuit using NdFeB permanent magnets. The collector has a small footprint of the size 12”x3”x6” and ran on a battery pack. The collector built on the HGPMS principle is highly selective toward particles comprising of paramagnetic and ferromagnetic composition[7], which eliminates significant downstream effort in preparing the same for composition analysis. Results from detailed model analysis and experimental measurement on the magnetic circuit reveal the existence of localized structures in the magnetic field density distribution. Time-resolved fluorescence data show that aerosol particles were rapidly captured by the structures, not by the peripherals of the magnetic circuit. For ferromagnetic particles of 50 nm or larger in size, the HGPMS technology would collect the particles with nearly 100% efficiency. The efficiency decreases following the decrease of particle size. The harvesting efficiency of the HGPMS technology appears to be primarily dependent on the particle magnetic moment instead of particle mixing. The internal instead of external makeup of the aerosol particle population determines the separation efficiency of the HGPMS collector.

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4IM.31

High Time Resolved Measurements of Ultrafine Particles, PM10, PM2.5, Nitric Oxides and Black Carbon at Berlin City.

MARKUS PESCH, Volker Ziegler, *Technical Director*

Although ultrafine particles account only for a little share in the total mass concentration, they are under a cloud of being harmful to health. For this reason an additional monitoring of this particle fractions´ exposure is absolutely necessary. First steps of continuous measurements of ultrafine particles have already been realized in high sophisticated systems like the Grimm EDM665 Wide Range Aerosol Spectrometer. Due to the temporal resolution of the integrated mobility spectrometer (SMPS) as well as it comparatively high costs it does not focus on area-wide monitoring of ultrafine particles.

A more competitive alternative for measuring the particle ambient exposure of ultrafine particles with high temporal resolution (1 second) is the combination of special environmental Condensation Particle Counter (CPC) in combination with a well-established Nafion drying system and an air conditioned mini-shelter. This GRIMM EDM465-UFP is absolutely qualified for continuous measurements of the ultrafine particle exposure and focus on hot- spot observations as well as on area-wide monitoring (e.g. background measurements). The device is performed for long term unattended measurements with low maintenance (1/months). Count efficiency, dryer performances and particle losses in the inlet pipe have been characterized comprehensively.

Measurements taken with the EDM465-UFP next to Berlin Zoo, Germany will be presented. The evaluation of the high time resolved data has been carried out in relation to local and regional sources and under different meteorological aspects. A condensation particle counter and a Laser spectrometer, placed at the measurement terrace of the Department of Environmental Chemistry, Technical University of Berlin, close to Berlin Zoo, is used to observe background concentration of ultrafine particles an PM values. Interesting correlations of UFP with PM10, PM2.5, NOx and black carbon will be shown.

4IM.32

A Method for Testing the Accuracy of the Hourly-Averaged PM2.5 Mass Concentration by Automated Measuring Systems for Continuous Monitoring with Laboratory Generated Aerosols. Yoshiko Murashima, HIROMU SAKURAI, *AIST*

We evaluated a method for testing $PM_{2.5}$ automated measuring systems for continuous monitoring ($PM_{2.5}$ systems hereafter) in the laboratory, with respect to the accuracy of the hourly-averaged mass concentration. While the accuracy of the daily-averaged mass concentration of $PM_{2.5}$ systems is tested and must be within a prescribed tolerance for qualifying for certification, there is no tolerance set for the accuracy of the hourly concentration. The accuracy of hourly concentrations is important in Japan, however, since hourly concentrations are used for issuing alerts by local governments when high $PM_{2.5}$ concentrations are expected. Testing the accuracy of hourly concentrations is not straightforward, though, since the method for testing the accuracy of daily concentrations, i.e., the comparison with the daily concentration determined by the reference filter/gravimetric method, is not applicable to hourly concentrations because of the lack of sufficient sensitivity. We propose a method for testing the accuracy of hourly concentrations that is to be performed in the laboratory, which uses laboratory-generated aerosols and a reference instrument that has a time resolution better than an hour. This method is reproducible and well-defined in comparison with methods with ambient aerosols. In this presentation, results from our experiments for validating the proposed testing method are reported.

Three types of $PM_{2.5}$ systems were tested. Two of them were beta attenuation monitors with Japanese certification (BAM-A and -B), and the other was a tapered element oscillating microbalance (TEOM). For reference measurement, we used two methods. One was a traditional filter/gravimetric method with two samplers as the primary standard, and the other was a scanning mobility particle sizer (SMPS) spectrometer as the secondary standard. The mass concentration by the SMPS was calibrated by the filter method. As test aerosols, we used two types of particles generated by the spray-drying method. One was an aerosol of 300-nm PSL spheres, and the other was a polydispersed aerosol of ammonium sulfate particles with mass mode diameter of about 120 nm. The particles were conditioned for concentration, humidity, and electrical charge, and then delivered to a manifold from which the tested $PM_{2.5}$ systems and references sampled.

We carried out two tests in the experiments. One was a test at a constant particle concentration of about 100 $\mu g/m^3$ for 3 hours. Two filter samplers gave reference 3-h average concentrations, which were compared to 3-h concentrations by the SMPS to determine correction factors for the SMPS for each particle type, i.e., PSL and ammonium sulfate. Hourly concentrations by the SMPS after correction with an appropriate correction factor thus determined were used as reference for evaluating the accuracy of hourly concentrations by the $PM_{2.5}$ systems. The agreement between the $PM_{2.5}$ systems and reference was generally good. BAM-B, however, showed large disagreements for the first hour of the 3-h measurement periods. The disagreement seemed to occur due to slow response of BAM-B. The hourly concentrations for the first hour by BAM-B seemed to be affected by the concentration before the 3-h periods, probably because the averaging time length that was set in the instrument was longer than an hour.

The other test was done at five concentration levels changed stepwise to evaluate the linearity of the $PM_{2.5}$ systems. The concentration levels were 10, 20, 40, 80, and 160 $\mu g/m^3$. Each concentration level was kept for 2 hours and the hourly concentrations of the second hour at each concentration level were compared with the hourly concentrations by the reference SMPS. The linearity was found fairly good for all of the $PM_{2.5}$ systems in the concentration range evaluated.

4IN.1

Understanding the Ice Nucleation Potential of Organic Sea Spray Aerosols. MARTIN WOLF, Lily Dove, Allison Coe, Maria Zawadowicz, Keven Dooley, Sallie Chisholm, Daniel Cziczo, *Massachusetts Institute of Technology*

The effects of atmospheric aerosols on cloud properties remain the largest source of uncertainties in predicting future climates. Processes of aerosol-induced ice nucleation affect the global radiative budget and hydrological cycle by influencing cloud formation, lifetime, albedo, and precipitation efficiency. Understanding the factors governing ice nucleation is therefore requisite to improving aerosol-cloud interactions in atmospheric models and reducing uncertainty in climate forecasts.

Atmospheric ice nucleation proceeds through processes of homogeneous and heterogeneous nucleation. In heterogeneous nucleation, an ice nucleating particle (INP) raises the temperature or lowers the ice supersaturation required to initiate ice formation. The organic components of sea spray aerosols (SSA) exhibit several qualities of effective INPs, such as such as hydrophilic functionality and the ability to increase porosity and surface roughness through glassy state phase transitions. In this study, we quantify the ice nucleation potential of laboratory generated SSA in the cirrus regime ($-60 \leq T \leq -40$ ˚C and $1.0 \leq S_{ice}$ 1.5). Nucleation potential is quantified by the temperatures and supersaturations required to initiate ice formation. NaCl and synthetic seawater were chosen as representative inorganic components of natural SSA, while aerosols generated from lysed cell cultures of the abundant and widespread phytoplankton Prochlorococcus were chosen as representative organic components of natural SSA. Deposition ice nucleation for particles generated from lysed plankton cultures initiated at ice supersaturations up to 30% lower than for purely inorganic particles, which activated in homogeneously.

We then investigated the effects of SSA composition and chemistry on nucleation. Organic enriched bubble film burst particles from lysed plankton cultures nucleated at lower ice saturations than inorganic enriched jet drop particles. We also used single component organic particles to explore the role of functionality in the nucleation of organic SSA. The deposition nucleation potential of lipids, saccharides, and proteins representative of natural marine organic matter was quantified. Lipids and oligosaccharides were overall ineffective depositional INPs, whereas polysaccharides and some amino acids were shown to mimic the effective nucleation behavior of aerosols generated from lysed cell cultures.

Finally, we present data from a recent field campaign in the Subtropical Atlantic Ocean, where Prochlorococcus is present in abundances up to 10^4 cells per mL of seawater. Organic microlayer and subsurface seawater samples were collected, aerosolized, and tested for nucleation potential in the cirrus regime.

Keywords: Sea Spray Aerosol, Ice Nucleation

4IN.2

The Influence of Dust Mineralogy on Its Aerosol Suspension Freezing Behavior. KRISTINA HÖHLER, Romy Ullrich, Thea Schiebel, Nadine Schittko, Barbara Dietel, Peter G. Weidler, Konrad Kandler, Ottmar Möhler, Thomas Leisner, *Karlsruhe Institute of Technology*

In mixed phase clouds, the freezing of individual cloud droplets is triggered by the presence of so-called ice nucleating particles (INPs). As this first ice formation usually is followed by a chain reaction of secondary ice multiplication processes, the abundance of these very rare aerosol species is critically for the initialization of precipitation and for cloud radiative properties.

Because of its high global atmospheric abundance, soil dust from arid regions is known to contribute significantly to INP concentrations, especially for freezing temperatures below -15°C. In past studies it was suggested that the immersion freezing behavior of this predominantly mineral dust can be described by a single parameterization disregarding the dust origin (Ullrich et al., 2017). On the other hand, some laboratory studies on suspension freezing behavior suggest that single mineralogical components, especially K-Feldspar, control the ice nucleating potential of the aerosols (Atkinson et al., 2013). This might imply the need for understanding the global distribution of aerosols with various compositions and the use of individual parameterizations for specific minerals in weather and cloud models.

In the INUIT09 campaign, organized at the AIDA (Aerosol Interaction and Dynamics in the Atmosphere) facility at KIT in Germany in July 2017, mineral dusts of different origin were carefully characterized according mineralogical composition and ice nucleation activity. Amongst other techniques, the new Ice Nucleation Spectrometer of the Karlsruhe Institute of Technology (INSEKT) was used to investigate the immersion freezing behavior of aerosol that was dry dispersed into a large vessel, sampled on filters and washed off. The construction of INSEKT was inspired by the design of the Colorado State University Ice Spectrometer developed by Hill et al. (2016), which enables the investigation of 50µl samples in 96-well PCR plates inserted in a temperature controlled aluminum block. INSEKT works with automated optical freezing detection during defined cooling ramps and can be used to study freezing events to temperatures as low as -27°C.

We will show first results on the immersion freezing behavior of eleven samples from different arid regions and discuss correlations with particle mineral compositions.

4IN.3

Isothermal Immersion Freezing Experiments Involving Mineral Dust: The Role of INP Surface Area. ASSAF ZIPORI, Daniel Knopf, Yinon Rudich, *Weizmann Institute of Science*

Ice nucleation in mixed phase clouds are still not well understood. This has many implications on the understanding of the radiative effects and rain formation in such clouds. Immersion freezing is considered to be the most important ice nucleation pathway in mixed-phase clouds, and recent field and modeling studies suggest a time-dependent ice nucleation process. Currently, two main approaches are used to describe immersion freezing: (1) The classical nucleation theory (CNT) that assumes a stochastic freezing process expressed by a heterogeneous ice nucleation rate coefficient (Jhet) that depends on surface area and time, and (2) a deterministic or singular (time independent) approach which is described by an ice active site density (Ns), which is determined by the surface area only.

It has been claimed that CNT fails to describe apparent varying freezing rates for isothermal experiments for single INP type. However, a recent study suggests that ice nucleation can be explained by a combination of stochastic uncertainty, when observing too little freezing events, and variation of INP surface area among droplets. We extend the experimental immersion freezing data set to test the effect of varying INP surface on immersion freezing using sufficiently large numbers of freezing events to render stochastic uncertainty negligible.

We present results of isothermal experiments using the WeIzmann Supercooled Droplets Observation on a Microchip (WISDOM). Using this setup, it is possible to analyze a large number of freezing events in each experiment, with a narrow droplet size distribution, thereby providing a good data set for analysis and parameterization. In addition, the INP efficiencies of minerals expressed as Jhet and Ns were also determined applying a constant cooling rate experiments. Those were followed by isothermal freezing experiments, where the temperature was held constant for up to three hours, for different temperatures. Jhet derived from constant cooling experiments were applied to describe the increase in the frozen fraction during the isothermal freezing experiments and for comparison with the Jhet derived directly from the isothermal freezing experiments. In the next step, the INP size distribution was examined in order to properly estimate the INP surface area distribution in the drops. By assuming a varying INP surface area distributed between the drops, the observed frozen fraction values in the isothermal freezing experiment could be described using a single value of Jhet for the applied temperature.

These experiments enhance our descriptive understanding of ice nucleation parametrization and classical nucleation theory. This will improve our ability to model primary ice nucleation in clouds for applications in cloud and climate models, with important effects on Earth’s radiation budget and the hydrological cycle.

4IN.4

Does Secondary Ice Processes in Mixed Phase Clouds More Important Than We Assume? ASSAF ZIPORI, Naama Reicher, Yigal Erel, Daniel Rosenfeld, Amir Sandler, Daniel Knopf, Yinon Rudich, *Weizmann Institute of Science*

It is generally assumed that secondary ice processes (SIP) influence the ice content in clouds that form in areas with low aerosol and ice nucleation particles (INP) concentration. However, in continental clouds, with high aerosol and INP concentrations, SIP are thought to be minor, and ice nucleation is assumed to be dominated by the INP concentration.

Here we combine field observations, laboratory measurements and model results to investigate the possible role of primary ice nucleation in continental, mixed phase, orographic clouds. Primary ice nucleation was quantified using the WeIzmann Supercooled Droplets Observation on a Microchip (WISDOM). Particles collected from rain samples were used to estimate the ice nucleation efficiency in the immersion mode. The immersion freezing results were compared with satellite-retrieved glaciation temperatures (Tg) and with an immersion freezing model, and used to examine the relative role of primary and secondary ice processes on cloud glaciation. In addition, the INP efficiency was also related to the particles' minerology.

We found that primary ice nucleation was controlled by K-Feldspar, although it was not the most abundant mineral. The role of SIP was assessed by comparing the observed Tg with the temperature where 50% of the drops froze in the WISDOM experiments (ΔT). This difference was minimal when the aerosols' concentration in the rain water was 10mg L-1. ΔT increased at lower aerosol concentration, suggesting that SIP were more effective due to larger droplets. At higher dust concentrations, ΔT increased possibly due to higher surface area available in cloud droplets compared to the WISDOM experiments. In addition, giant cloud condensation nuclei could also have initiated SIP by forming large droplets at early cloud growth stages. Using a simple model of primary ice nucleation, the calculated glaciation temperature was compared with the observed Tg. Although the model design favored primary ice nucleation, it did not explain the observed Tg from the satellite.

Our results show a direct relation between the drops size and the importance of SIP. In addition, we show that SIP is not limited to clouds with low aerosols concentration, but exist also in continental clouds, which were assumed to be less prone to SIP. This is due to large dust aerosols that are carried to the clouds during severe dust storms. These large dust aerosols can act as giant cloud condensation nuclei that freeze at relatively high temperatures, and initiate SIP. Our results emphasize the importance of SIP on Earth's radiation budget and its influence on global climate, as it is larger than usually assumed.

4IN.6

Nanoscale Ice-Nucleating Particles in Waterbodies in an Agricultural Area. HEIKE WEX, Kathryn A. Knackstedt, Bruce Moffett, Susan Hartmann, Janine Fröhlich-Nowoisky, Thomas Hill, Sarah Grawe, Robert Michael McKay, *Institute for Tropospheric Research, Germany*

Ice nucleating particles (INPs) are a neglected, but integral component of the water cycle. Abundant INPs were identified from surface waters of both the Maumee River and Lake Erie with freezing profiles spanning a temperature range tested from -30°C to -20°C. River INPs were largely attributed to biogenic macromolecules, based on their characterization showing heat denaturation of ice activity and size-fractionation of the activity using a 0.2 µm membrane. Higher concentrations of INPs were found in river samples compared to lake samples. However, the latter showed a broader increase in the freezing profile, pointing towards a different population of INPs being present in the lake.

Seasonal analysis of INPs that were ice active ≥ -10°C (INP_{-10}) showed their concentration to correlate with river discharge, suggesting a watershed origin of these INPs, a characterization supported by analysis showing similar ice nucleating signatures derived from the river and the soil fungus Mortierella alpina suggesting that fungal INPs may dominate the INP population of the river. Aerosols derived from turbulence features in the river can include INP_{-10} that may potentially influence regional weather. INP_{-10} contained within aerosols generated from a weir spanning the river ranged in concentration from 1-11 INP m^{-3} which represented a fold-change of 3.2 over average INP_{-10} concentrations sampled from aerosols at control locations.

4IN.9

Single-Particle Mixing State and Mineralogy of North African Dust: A Comparison of Ambient Transported Dust with Laboratory Generated Proxies. NICHOLAS MARSDEN, Romy Ullrich, Ottmar Möhler, Paul Williams, Michael Flynn, James Allan, Hugh Coe, *University of Manchester*

Mineral dust has been the subject of many laboratory simulations of ice nucleation (IN) due to the potential for these particles to act as ice-nucleating particles (INP). In many studies, the mineralogy of single particles has been found to influence the conditions at which ice is formed and is therefore an important parameter in this type of experiment. Furthermore, the internal mixing state, such as the coating with sulphate and organics, can alter the characteristics of INP and is also an important consideration. Therefore, the characterisation of single-particle mineralogy and mixing state of mineral dust is an important for the modelling of IN at atmospherically relevant conditions.

In this study, we present the online analysis of the fine fraction (<2.5µm) of North African dust using single-particle mass spectrometry (LAAPTOF, AeroMegt GmbH), a technique that has a unique ability to make online measurements of single-particle composition and mixing state at high temporal resolution. Using novel data evaluation methods, we evaluated the number concentrations of felsic, illite and kaolinite clay particles and the internal mixing with organic, inorganic and biological material in commonly used mineral dust proxies including; crushed microcline feldspar, synthetic illite NX, natural soil from the North-West margin of the Sahara, and natural soil from the Sahel region. The materials were sampled from the AIDA chamber, Karlsruhe Institute of Technology, prior to ice formation during the INUIT09 campaign July 2017. The data is compared to the composition of transported dust measured with the same instrument in the marine boundary layer at Praia, Republic of Cabo Verde, during the ICE-D campaign in August 2015.

The similarities and differences of the ambient dust compared to the laboratory generated proxies will be discussed with reference to the implications of dust modification during transport and the atmospheric relevance of commonly used mineral dust proxies.

4IN.10

Cleaning up Our Act: Assessment of Background Freezing Caused by Impurities and Substrates and Strategies to Reduce These Interferences in Droplet Freezing Assays.

Michael Polen, Thomas Brubaker, Josh Somers, Perry Cheng, RYAN SULLIVAN, *Carnegie Mellon University*

Droplet freezing techniques have been utilized for decades to measure the concentration of ice nucleating particles (INP) and assess the freezing properties of atmospheric particles. However, these methods suffer from contamination issues, especially in regards to impurities in the water or on the substrates used that induce freezing at temperatures warmer than the homogeneous freezing limit. Published results often do not present a sufficiently in-depth discussion of how the pure water was generated or its quality, or an assessment of background freezing due to surface interactions or matrix impurities. We present a detailed assessment of the droplet freezing temperature spectra and inferred INP concentrations obtained using different substrates in the CMU cold stage system, as well as the effects of different approaches to water purification and the resulting matrix impacts on the background freezing spectrum. We have found that bottled HPLC water along with filtration provides the lowest background signal and the most consistent pure water freezing spectra, though many in the ice nucleation community use Milli-Q generated water instead. Typical Milli-Q purification systems do not filter particles smaller than 200 nm, which could explain the inconsistent freezing spectra we observed. We have also observed the quality of the Milli-Q produced water to change suddenly with use. Substrates tested include silicon wafers, Vaseline, gold-coated surfaces, hydrophobic cover slips, and polydimethylsiloxane polymer. Our findings suggest that gold-coated substrates induce freezing at the lowest temperatures, while Vaseline consistently causes samples to freeze at higher temperatures. However, nearly all substrates induce freezing at higher temperatures than previous literature suggests, and warmer than the homogenous freezing temperature threshold. We also lay out our recommendations for future ice nucleation studies to present, in detail, how different research groups control for contamination and background freezing of a rare phenomenon that is highly sensitive to contamination. In this vein, we encourage the community to regularly publish droplet volume-normalized ice nucleating particle concentrations for pure water tests, as well as the raw droplet freezing temperature spectra. This will enable a direct comparison between methods so the community can identify the best practices and materials for droplet freezing techniques.

4IN.11

Effects of Atmospheric Chemical Aging on Biomass Burning Aerosol Composition and Ice Nucleating Properties. LYDIA JAHL, Michael Polen, Leif Jahn, Thomas Brubaker, Ryan Sullivan, *Carnegie Mellon University*

Biomass burning is a major global source of aerosol pollution that comprises nearly 80% of the total carbonaceous aerosol burden and 2700 Gg of black carbon emissions per year. The ability of some aerosol particles to nucleate ice was once thought to only occur in mineral dust and biological particles, but recent studies found that some types of biomass burning aerosol (BBA) can also nucleate ice and cause the glaciation of clouds. Cloud glaciation causes changes in the evolution of a cloud's properties and structure by initiating precipitation, influencing atmospheric chemical reactions, changing cloud lifetime and size, and altering the cloud's radiative forcing. We seek to understand what chemical properties of the aerosol particles might explain the nucleation of ice at mixed-phase cloud temperatures. Furthermore, many studies focus on the ice nucleating abilities of fresh, unaged aerosol that may not represent realistic BBA, which experiences significant chemical processing and aging. Therefore, we explored the relationships between the ice nucleating abilities and chemical properties of authentic biomass burning aerosol that we chemically aged in an environmental chamber.

We burned biomass fuels that are commonly consumed in wildfires and prescribed burns such as sawgrass, birch, and black needlerush to fill an environmental smog chamber with biomass burning aerosol smoke. The aerosol was aged using three different chemistries: hydroxyl radical aging by injection of nitrous acid with UV lights, dark ozonolysis, and by hydroxyl radical aging of aerosol particle surfaces only by first passing the aerosol through a thermal denuder to remove organic components. In several systems, hydroxyl radical aging was found to enhance the aerosol's ice nucleation properties. For example, the ice active site density of cutgrass BBA increased by half an order of magnitude following oxidation corresponding to a 10% increase in the O:C ratio of the aerosol. However, this was not an effect consistently observed for all biomass fuels tested. The chemical composition of the aerosol was analyzed using two single-particle mass spectrometers (SP-AMS and LAAPTOF), and the particles were collected on filters for SEM/EDX analysis and to determine their ice nucleating abilities. We analyzed the ice nucleating properties of the biomass burning aerosol on a cold plate using two different droplet generation techniques: droplets directly pipetted into an oil bath and droplets stored and created on a custom microfluidic chip. We will present our findings on the changes in the aerosol's composition following chemical aging, and will correlate the ice nucleating abilities of different plant species' fresh and aged emissions to their aerosol chemical composition.

4IN.12

Responses of Mixed-Phase Cloud Condensates and Cloud Radiative Effects to Ice Nucleating Particle Distributions in DOE E3SM model.

YANG SHI, Xiaohong Liu, Mingxuan Wu, Kai Zhang, *University of Wyoming*

Mixed-phase clouds frequently observed in the Arctic and mid-latitude storm tracks have substantial impacts on the global energy budget, precipitation, and climate. In this study, we first implement two empirical ice nucleation parameterizations (Niemand et al. 2012 and DeMott et al. 2015) in the DOE Energy Exascale Earth System Model version 1 and version 0 (E3SM v1 and v0). For both of the two model versions, model simulated ice nucleating particle (INP) concentrations using Niemand et al. and DeMott et al. are compared with the simulation using default classical-nucleation-theory-based ice nucleation scheme (CNT). We find that Niemand et al. presents significantly higher (a factor of 3) INP concentrations than DeMott et al. and CNT near the dust source regions. Moreover, because of the more efficient aerosol (dust) transport to the Polar Regions, E3SM v1 shows around 100 times more INP than E3SM v0 at the Arctic regions for all of the three parameterizations. This also causes a 20% difference in liquid water path and a 10% difference in cloud radiative forcing (shortwave and longwave) in the Arctic regions between the three ice nucleation shcemes in E3SM v1, which are not seen in E3SM v0. Finally, the dust burdens from E3SM v1 and v0 are compared with CALIPSO data and the surface observation at the Alert station in Canada.

4IN.13

Activation of Intact Bacteria and Bacterial Fragments Mixed with Agar as Cloud Droplets and Ice Crystals in Cloud Chamber Experiments. KAITLYN J. SUSKI, David Bell, Naruki Hiranuma, Ottmar Möhler, Dan Imre, Alla Zelenyuk, *Pacific Northwest National Laboratory*

Bacteria has been extensively studied for its ability to nucleate ice in the immersion regime at modestly supercooled temperatures. Previous studies have shown that while whole bacteria cells are efficient ice nucleating particles (INPs), smaller bacterial fragments and even individual proteins from bacteria can also serve as INPs. Experiments conducted at the Aerosol Interaction and Dynamics in the Atmosphere (AIDA) cloud chamber at the Karlsruhe Institute of Technology (KIT) investigated the ice nucleation activity of two strains of cultivated bacteria (pseudomonas syringae and PF CGina) by forming a cloud via expansion at temperatures between -5 and -12 °C. We find that bacterial fragments mixed with agar growth media activate as cloud condensation nuclei (CCN) and INPs, while intact bacteria cells were not observed in cloud droplet and ice crystal residuals.

Cloud droplet residuals were sampled using a pumped counterflow virtual impactor inlet (PCVI) and ice crystal residuals were sampled using an ice-selecting PCVI (IS-PCVI). A single particle mass spectrometer (miniSPLAT) was used to characterize the size and chemistry of aerosol particles and cloud residuals. The aerosol in the AIDA chamber before and after the expansions had a bimodal size distribution with agar mixed with bacterial fragments comprising the smaller size mode and whole bacteria cells making up the larger size mode. Three expansions were performed with two bacteria strains and all expansions showed that the cloud droplet residuals had the same size distribution and mass spectral signatures of the bacteria fragments mixed with agar. Additionally, the ice crystal residuals were also composed of bacteria fragments mixed with agar. Due to the fact that an immersion mode INP must first become incorporated into a cloud droplet, whole bacteria cells were unable to serve as INPs in these experiments due to their limited CCN activity.

Previous studies have suggested that bacteria can range from hydrophobic to slightly hydrophilic due to the varying makeup of the bacteria cell wall. Thus, if bacteria are not hygroscopic, it could explain why they are less CCN active than bacteria fragments that are not completely enveloped in a cell wall and are mixed with a very hygroscopic material, in this case agar. These results suggest that in clouds where water vapor is limited, competition for water vapor between weakly hygroscopic intact bacteria and other more hygroscopic particles could result in a negligible amount of intact bacteria serving as CCN and INP in the immersion mode. In the laboratory, bulk immersion freezing measurements do not capture this competition for water vapor as particles are submerged in a well of water or a water droplet artificially overcoming this barrier to CCN activation. Also, if agar is adding to the hygroscopicity of the bacteria fragments in cultivated bacteria and enhancing their CCN and thus immersion INP activity, the role of agar must be quantified to understand these laboratory data in relation to real clouds.

4IN.14

Ice Nucleation Activity of Glassy Soil Organic Particles under Cirrus Conditions. SWARUP CHINA, Daniel Veghte, Joseph Charnawskas, Johannes Weis, Kaitlyn J. Suski, Gourihar Kulkarni, Bingbing Wang, Peng Lin, Alla Zelenyuk, Mary Gilles, Daniel Knopf, Alexander Laskin, *Pacific Northwest National Laboratory*

Glassy soil organic particles can play a significant role in heterogeneous ice nucleation under cirrus cloud conditions. Our previous study showed formation of airborne soil organic particles (ASOP) from the soil surface after intensive rain events in the Southern Great Plains (SGP), Oklahoma. In this study we collected aliquots of 'soil organic matter brine' from a puddle created by the rain events to generate spherical solid ASOP-like particles under laboratory conditions. Chemical imaging and micro-spectroscopy analysis of soil organic particles are performed to characterize their physico-chemical properties. Furthermore, molecular characterization and elemental composition analysis of particle constituents are performed by high-resolution mass spectrometry. We utilize a custom-built ice nucleation cell, interfaced with an Environmental Scanning Electron Microscope (IN-ESEM platform) operated at temperature and relative humidity relevant for cirrus cloud formation to investigate ice nucleation propensity of these laboratory generated soil organic particles. We show dynamic microscopic observations of ice nucleation events on individual submicron size soil organic particles via deposition mode. Our results show that relative humidity with respect to ice of soil organic particles is similar for to that of Suwannee River Fulvic Acid particles. Overall, our results show that soil organic particles promote ice formation under cirrus conditions.

4IN.15

Chemistry of Ice Nucleating Particles in Summertime Urban/Marine Conditions. MARIA ZAWADOWICZ, Michael Roesch, Martin Wolf, Daniel Cziczo, *Massachusetts Institute of Technology*

Formation of ice in the atmosphere depends critically on the availability of ice nucleating particles (INPs). Field and laboratory measurements indicate that a small fraction of tropospheric aerosol particles are efficient INPs and that their chemistry is distinct from that of bulk aerosol. Although the specific chemical qualities that govern ice nucleation efficiency remain uncertain, mineral dust, metallic anthropogenic particles and certain species of bioaerosol have been shown to be efficient INPs in field and laboratory studies. In this experiment, a single particle mass spectrometer (Particle Analysis by Laser Mass Spectrometry, PALMS) was coupled to a continuous flow diffusion chamber (Spectrometer for Ice Nuclei, SPIN) using a pumped counterflow virtual impactor (PCVI). The resulting instrument combination allows direct measurement of ambient INPs under a range of temperature and saturation conditions and simultaneous characterization of chemical composition of their residuals. The technique was validated in the laboratory and deployed in downtown Cambridge, MA to sample air masses of continental and marine origin, strongly influenced by Boston-area pollution. Temperature and saturation conditions consistent with deposition and immersion ice nucleation modes were used.

4IN.16

Effect of Solutes on Ice Nucleation Efficiency of Feldspar. JINGWEI YUN, Jon Davidson, Allan Bertram, *University of British Columbia*

Mineral dust particles are abundant in the atmosphere. When these particles are immersed in cloud droplets they can catalyze the nucleation of the ice phase. One type of mineral dust particle that is especially good at nucleating the ice phase is microcline (a potassium-rich feldspar) (Atkinson et al., 2013). When mineral dust particles are immersed in cloud droplets, organic and inorganic solutes are typically present. Our work focuses on the effect of these organic and inorganic solutes on the freezing properties of microcline immersed in droplets. Experiments were carried out with the droplet freezing technique as described in Whale et al. (2015). A range of organic and inorganic solutes was studied including a series of inorganic nitrates. The results show that the studied solutes have a larger effect on the freezing properties of microcline than expected from freezing point depression caused by solutes. Results from these studies will be presented and discussed.

4IN.18

Effect of Surface Geometry on Heterogeneous Ice Nucleation. Olli Pakarinen, Golnaz Roudsari, EVGENI ZAPADINSKY, Hanna Vehkamäki, *University of Helsinki*

Understanding the way in which ice forms is of great importance to many fields of science. Pure water droplets in the atmosphere can remain unfrozen to nearly -40º C. Crystallization of ice in the atmosphere therefore typically occurs in the presence of aerosol particles, such as mineral dust, soot or organic particles. These ice nucleating particles (INPs) cause heterogeneous ice nucleation at clearly higher temperatures than possible through homogeneous ice nucleation. Therefore, a better understanding of how the various types of aerosol particles present in the atmosphere affect ice nucleation (IN) in clouds would improve our ability to measure, model and parameterize the key processes related to ice- and mixed-phase cloud formation, and would advance the field of atmospheric science.

Experiments have shown in great detail what is the IN activity of different types of compounds, and recently also clarified the importance of small surface features such as surface defects. The molecular-scale processes responsible for ice nucleation are still not well known, however, and difficulties in atomic-scale characterization of complex and imperfect surfaces means that a full understanding of these processes from solely experimental evidence is still a distant goal. In recent years, several computational studies have been published on heterogeneous ice nucleation, advancing our understanding of the details of ice nucleation in many materials. The role of defects has been studied less, but recently the importance of feldspar microstructure and different crystallographic faces of feldspar were shown to be responsible for IN activity of feldspars (Kiselev et al., 2017). Simulations also showed enhanced ice nucleation efficiency in confined geometry such as wedges or pits (Bi, Cao and Li, 2017).

We are studying these topics by utilizing the monatomic water model (Molinero and Moore, 2009) for unbiased molecular dynamics (MD) simulations, where a system including a defected surface, such as pyramidal pits, steps or surface cracks, immersed in water, is cooled continuously below the melting point over tens of nanoseconds of simulation time and crystallization is followed.

Results of simulations on pyramidal pits on Si (100) surfaces, for example, show a clear ($\Delta T > 10$º C) enhancement of ice nucleation compared to flat Si (100) or Si (111) surfaces. Understanding the enhanced activity in such confined geometry may lead to characterization of active sites on some ice nucleating materials, as well as to development of optimal cloud seeding materials.

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4IN.19

Adsorption Nucleation Theory for Ice Formation from the Vapour Phase. ANDRÉ WELTI, Ana A. Piedehierro, Yrjö Viisanen, Annele Virtanen, Lise Deschutter, Outi Meinander, Ari Laaksonen, *Finnish Meteorological Institute*

The recently developed framework of adsorption nucleation is applied to describe ice formation from the vapour phase on insoluble particles. The theory (Laaksonen, 2015; Laaksonen and Malila, 2016) is based on a combination of the Frenkel-Halsey-Hill (FHH) adsorption isotherm and the Kelvin equation, and it describes the adsorption of water in spherical clusters on a substrate and predicts, in dependence of substrate properties the critical saturation at which clusters reach a stable size. These ice clusters then serve as centres for ice to grow into a macroscopic ice crystal. The theory has previously been applied successfully to predict onset conditions of ice nucleation triggered by several soot species at low temperatures (Laaksonen et al., 2018).

Here we investigate if the theory works equally well for ice formation on natural mineral dust samples including Arizona Test Dust and Islandic dust of volcanic origin. Input parameters for the adsorption nucleation theory (contact angle and FHH adsorption parameters between water and the substrate) are determined experimentally for the same samples the ice nucleation efficiency has been measured.
The theoretical predictions of the adsorption nucleation framework and of classical nucleation theory are contrasted with measurements from the literature, so that the comparison serves as a test of correctness of the theories.

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4IN.20

A Microfluidic Ice Nucleating Particle Counter for Continuous Measurements. Ali Mohammadi Nafchi, Gavin McMeeking, ANDREW METCALF, *Clemson University*

Droplet freezing experiments have been of interest for many years because of the difficulty in describing ice formation in the atmosphere with a single theoretical model. The majority of these experiments are conducted in a chamber or flow tube on a population of particles to determine parameters necessary for modeling ice nucleation in the atmosphere. Recent advancements can examine freeze-thaw cycles in single droplets on a microscope cold stage using oil immersion techniques. The techniques currently employed by the community are typically only capable of batch measurements, and the sum of many measurements represents the behavior of a population of ice nucleating particles.

In this talk, we present a new technique to provide continuous measurements of droplet freezing and thawing events, with the ultimate goal of continuously counting ice nucleating particles (INP). Droplet microfluidics are combined with on-chip temperature measurements and a multi-zone cold stage to continuously generate, freeze, and thaw liquid droplets. Temperature control to at least -40 degrees C will allow homogeneous freezing of pure water droplets with rapid repeatability. The microfluidic device includes an embedded platinum resistance temperature detector array which precisely measures temperature at 19 points along the fluid flow channel. The microfluidic device sits on a temperature control block which has 7 discrete temperature zones capable of causing a temperature gradient along the fluid flow. Multiple temperature zones allow hot-cold-hot hysteresis cycles to be observed in single droplets. Initial experiments with this new platform include high-speed observations of droplet freezing at a range of temperatures and INP concentrations.

4IN.22

Probing the Identity of the Ice Nucleating Particles (INPs) in a Boreal Environment. MIKHAIL PARAMONOV, Saskia Drossaart van Dusseldorp, Zamin Abdulali Kanji, *ETH Zürich*

Ice nucleation is an important pathway for cloud formation and initiation of precipitation in the atmosphere, thus affecting the Earth's hydrological cycle, energy and radiative balance (Mülmenstädt et al., 2015). It has been shown that a significant fraction of precipitating clouds in various environments contains ice, e.g. both in the tropics (Lau and Wu, 2003) and in the Nordic countries (Sporre et al., 2014). However, in many cases, the exact identity of an ice nucleating particle (INP) in a particular environment, as well as the properties that make an atmospheric INP an efficient one are still not fully understood (Kanji et al., 2017).

A ubiquitous aerosol particle species, the effect of which on atmospheric ice nucleation has not been thoroughly investigated, is the secondary organic aerosol (SOA). Boreal forest, which covers approximately 8% of the world's land area, is a significant source of SOA in the atmosphere. Therefore, an intensive measurement campaign, HyIce2018, is planned at the SMEAR II (Station for Measuring Ecosystem-Atmosphere Relations) boreal site in Hyytiälä Forestry Field Station in southern Finland (Hari and Kulmala, 2005). The measurement campaign is an international collaborative effort, involving several research institutions and various ice nucleation measurement techniques, supplemented by aircraft and tethered balloon, as well as the comprehensive network of aerosol- and meteorology-related continuous measurements deployed at the site. ETH Zürich will participate in the campaign in February-March of 2018 for approximately six weeks.

Continuous ice nucleation measurements will be conducted by the Portable Ice Nucleation Chamber (PINC) at a temperature of 242K in condensation freezing mode (i.e. above water saturation). The expectedly low INP concentrations at the site will be enhanced by a powerful aerosol particle concentrator, which can increase the particle number concentration by as much as a factor of 25. Besides INP number concentrations measured by PINC, the chemical composition of INP will be deduced from mass spectrometry, as well as from measurements of biomass burning and biological fluorescent particles. The participation of several research groups will also allow for an intercomparison of the deployed ice nucleation measurement techniques.

HyIce2018 is expected to be the first measurement campaign aiming at quantifying and qualifying the ambient INPs in a boreal environment. The planned measurement activities are expected to shed light on the identity of the INPs and the effect of SOA, biomass burning and biogenic aerosol particles on atmospheric ice nucleation.

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4MD.1

Hyperthermic Intracavitary Nanoaerosol Therapy (HINAT) - a Promising Approach to Treat Peritonealcarcinomatosis.

Daniel Göhler, Stephan Große, LARS HILLEMANN, Alexander Bellendorf, Thomas A. Falkenstein, Mehdi Ouaissi, Jürgen Zieren, Michael Stintz, Urs Giger-Pabst, *Technische Universität Dresden*

Pressurized Intraperitoneal Aerosol Chemotherapy (PIPAC) is an upcoming approach for the treatment of end-stage patients suffering on advanced peritonealcarcinomatosis. During conventional PIPAC (cPIPAC), a chemotherapeutic solution is aerosolized by a single-fluid nozzle (called micro injection pump MIP$^{®}$) within the capnoperitoneum (i.e., inflated peritoneum with an overpressure of 1.6 kPa = 12 mmHg based on carbon dioxide). This kind of drug delivery (Solaß et al. 2012) circumvents several problems (e.g. adverse effects, systemic intolerance, ineffective drug delivery) accompanied to other established therapeutic methods (e.g. intraperitoneal resection, systemic chemotherapy or intraperitoneal liquid chemotherapy). But recently performed granulometric analyses on the aerosol of cPIPAC revealed a high optimization potential (Göhler et al. 2017a).

Thus a new PIPAC method (Göhler et al. 2017b), called Hyperthermic IntraCavitary NanoAerosol Therapy (HINAT), was developed to improve the homogeneity as well as the effectivity of drug deposition over the whole peritoneum. HINAT provides a nanometer-sized, unipolar-charged and hyperthermic aerosol for intracavitary use based on extracavitary aerosol generation (i.e. atomization by a two-fluid nozzle and immediate separation of coarse droplets) with subsequent aerosol conditioning.

The performance of both HINAT and cPIPAC were characterized in a comprehensive testing program, which comprised ex vivo granulometric analyses (laser diffraction spectrometry, time of flight spectrometry, differential electrical mobility analyses, condensation nuclei counting) for aerosol characterization, in post mortem swine analyses (scintigraphic peritoneography, fluorescence microscopy) for the characterization of spatial drug distribution and in-tissue drug penetration and in vivo proof of concept analyses in anesthetized swines.

Results show, that HINAT provides despite a hundreds times lower liquid drug flow rate a 25 times higher droplet generation rate than cPIPAC with a quasi-uniform deposition profile over the whole peritoneum. At a 3 times lower dose of a chemotherapeutic substance, the drug penetration depth of HINAT was found to be two times higher than the one for cPIPAC. Further information on the HINAT method and even more detailed results will be presented.

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4MD.2

Analysis of Xenon Mass Transfer from Human Upper Airway to Systemic Regions using a Hybrid CFD-PBPK Model.

AHMADREZA HAGHNEGAHDAR, Jianan Zhao, Max Kozak, Patrick Williamson, Yu Feng, *Oklahoma State University, Stillwater, OK, USA*

Administrating incorrect doses of conventional anesthetic agents through the pulmonary route can cause potential health risks such as blood coagulation, platelet dysfunction, and deteriorating organ function. As an alternative, Xenon induces negligible impact on the cardiovascular system and also provide a neuroprotective effect, hemodynamic stability, and fast recovery. However, the inhalation still needs to be carefully monitored and controlled to avoid health risks caused by overdosing patients in unconsciousness. Thus, high-resolution lung absorption and whole-body translocation data are in critical need to fully understand how to administrate the gas via inhalation and coordinate with the patient to accurately control the dose. Clinical studies are not able to provide accurate dosimetry data due to their limited operational flexibility and imaging resolution. Therefore, a Computational Fluid Dynamics (CFD) model was employed in this study to simulate the transport and absorption of the inhaled Xenon which is connected with a Physiologically Based Pharmacokinetic (PBPK) model to predict the translocation into the systemic regions. To study the effects of different breathing patterns on Xenon transport dynamics and the concentration within the plasma and important organs, two inhalation durations (2 sec and 1.5 sec) were selected for each breathing cycle. Averaged inhalation flow rate is fixed at 3L/min to represent adults at rest. As this study only simulate inspiratory phase, a 1-sec holding time was applied to represent the expiratory phase. Simulations were performed in a subject-specific human upper airway configuration from mouth to G6. Our numerical results show that with the accurate lung uptake predictions obtained from the CFD model, the hybrid CFD-PBPK model generates more precise trends compared to simple PBPK models. In both cases, the concentrations increase with time before reaching a plateau after about 20 minutes. For 2-sec and 1.5 sec inhalation durations, the maximum values of Xenon uptake concentration during one single inhalation are approximately 0.1 and 0.07 mol/L respectively. The comparison indicates that higher uptake concentration of Xenon occurs with the long inhalation duration. Furthermore, the parametric analysis indicates that the plasma concentration of Xenon is significantly higher with the long inhalation duration. In conclusion, breathing pattern can significantly influence the Xenon uptake in the human body, which can be utilized as a critical factor to be coordinated by clinicians to achieve the optimized Xenon dose.

4MD.3

Aerosol Based Nanoscale Material Synthesis, Surface Engineering and Delivery to the Brain. RAMESH RALIYA, Nathan Reed, Debajit Saha, Dezhuang Ye, Tandeep Chadha, Hong Chen, Barani Raman, Pratim Biswas, *Washington University in St. Louis*

The brain is shielded by a group of parenchyma cells connected by tight junctions to protect the organ from foreign substances. The protecting layer of these cells, known as blood-brain barrier (BBB), creates an obstacle to the delivery and translocation of drugs to the brain. Current practices such as invasive delivery or non-invasive nasal droplet are limited either by a high risk of brain damage or slow and low volume delivery. In this study, we investigate a non-invasive approach, generating an aerosol suspension of ultra-small particles that can be delivered to the brain relatively faster than current medical practices. We used aerosol atomizers such as electrospray and Collison nebulizers to generate particles in the size range between 5 and 150 nm while maintaining particle properties and its uniform size distribution. The real-time particle size was measured by scanning mobility particle sizers. We have successfully tested the delivery of 5 nm gold particles to the locust brain and quantified particle delivery/uptake in the brain using inductively coupled plasma-mass spectroscopy. Building on this work, focused ultrasound technology is used for enhanced targeted delivery of nanoscale materials in the brain, potentially for brain cancer treatment. Such particles can be used as drug delivery vehicles, however, this would require a detailed investigation into the transport and delivery mechanism.

4MD.4

Pores of Kohn: Forgotten Alveolar Structures and Potential Aerosol Generators? MICHAEL OLDHAM, Owen Moss, *Altria Client Services LLC*

Analysis of aerosols in human and animal exhaled breath has identified numerous compounds from the deep lung, including proteins and surfactant constituents. Some mechanisms like coughing or surfactant/mucus plugs have been proposed to explain the presence of these exhaled deep lung constituents. However, these proposed mechanisms do not explain their presence, during normal breathing. Furthermore, current deterministic and computational fluid dynamic models do not provide insight into the means of generating such aerosols. This work explores the possibility that deep lung aerosols might be generated as a normal function of the opening of pores of Kohn.

Pores of Kohn are between-alveoli channels that have been found in numerous species including humans. Initially, pores of Kohn were thought to provide collateral ventilation to prevent excessive localized alveolar pressure. However, currently they are thought to provide collateral ventilation only under extreme conditions of alveolar duct or terminal bronchiole blockage. Additionally the pores are hypothesized to be fluid filled connections between alveoli, reservoirs for surfactant, portals for macrophage movement, and structures that are initially damaged (during development of emphysema when individual alveoli erode and seem to merge) in empheysema.

We reconsider a possible mechanism by which the pores of Kohn might open under normal breathing conditions. During inhalation alveolar tissue stretches, causing pore diameter to increase in spite of resistance from the surface tension of fluid filling the pore. Pore diameter continues to slowly increase until the meniscus at either end of the pore touch thus forming a thin unstable film. When this film randomly breaks during inspiration, the fluid surface tension now contributes to pore expansion. Furthermore, when the fluid film breaks an aerosol is formed.

The instability in the surfactant film, due to change in diameter of a pore of Kohn, results in opening of the pore following breakage of the film -- which can generate aerosols containing surfactant constituents. To more accurately calculate lung deposition and aerosol generation, pores of Kohn should be integrated into deterministic and computational fluid dynamic models.

4MD.5

Characterization of Airspace Dimension Assessment with Nanoparticles (AiDA) on a Large Population and Relation to Anthropometry and Lung Function Parameters. JONAS JAKOBSSON, H Laura Aaltonen, Hanna Nicklasson, Sandra Diaz, Per Wollmer, Jakob Löndahl, *Lund University*

Introduction

Airspace Dimension Assessment (AiDA) is a technique to assess airspace dimensions in the distal lung by measuring the recovery of inhaled nanoparticles (Löndahl et al. 2016, Jakobsson et al. 2016). It has previously been shown that the average diffusion distances, corresponding to effective airspace dimensions, can be inferred by measuring the half-life time of inhaled nanoparticles (Löndahl et al. 2016). It has also been suggested that estimated particle recovery after a hypothetical measurement without breath-hold (called the intercept) may hold additional information about individual lung features related to the conducting airways.

The aim of this work was to investigate the characteristics of the AiDA technique and the relation of the AiDA parameters to anthropometry and lung function parameters in a large population of mostly healthy subjects.

Method

Nineteen healthy subjects performed measurements of recovery of inhaled nanoparticles for breath-holding times between 5 and 20 s and volumetric sample depths between approx. 200 and 5000 mL. A simplified protocol, measuring recovery at a fixed (1300 mL) sample depth and breath-holding times between 5 and 10 s was performed by a larger group (n = 668). The measurements were performed with monodisperse 50 nm polystyrene nanospheres.

All subjects underwent a detailed investigation of lung function, including measurement of vital capacity (VC), forced expiratory volume in 1 s (FEV_1), lung diffusing capacity for carbon monoxide ($D_{L,CO}$) and forced oscillation technique (FOT), which gives information about respiratory resistance and reactance. The larger group also underwent a computed tomography (CT) scan of the lungs, to detect and quantify respiratory disease.

Characteristics of the derived airspace dimensions and the intercept (zero breath-hold recovery) were analysed in detail for the smaller group. Statistical analysis comparing AiDA to anthropometry and clinical lung function parameters was performed for the larger group to elucidate the AiDA parameters relation to established clinical techniques.

Results

The data from the smaller group showed that the derived airspace dimensions showed reasonable agreement with lung models based on histological measurements. The dimensions are root mean square (RMS) diameters of the airspaces and therefore larger than a normal arithmetic mean. The data also showed that both the airspace dimension and intercept were highly reproducible with sufficient sensitivity to reflect individual lung morphology.

The statistical analysis showed that the airspace dimensions correlated mainly with age, $D_{L,CO}$ and FEV_1/VC while the intercept correlated mainly with height, VC, FEV_1 and FOT. Importantly, airspace dimensions and intercept did not correlate strongly (n.s. for n = 19), (p =.02, r = -.09 for n = 668). Significant differences were detected between smokers (n = 101) and non-smokers (n = 570) ($p < 0.00011$ for intercept, $p < 0.0068$ for airspace dimensions) and between subjects with emphysema (n = 58, assessed with CT) and healthy subjects (n = 604), ($p < 0.0023$, $p < 0.0000000002$) for intercept and airspace dimensions, respectively.

Conclusion

The results show that the AiDA-derived airspace dimension and intercept convey independent information about individual lung properties. They further suggest that AiDA may have sensitivity to lung abnormalities (such as caused by smoking and respiratory disease); however studies including more subjects with respiratory disease are needed to evaluate the clinical value of the technique.

This work was supported by Swedish Research Council, Vinnova, EU EuroNanoMed, The Swedish Heart and Lung Foundation and the Crafoord foundation.

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4MD.6

Predicting Local and Systemic Distributions of Inhaled Budesonide Powders using In Vitro Experiments Combined with Numerical Modeling. CONOR A. RUZYCKI, Brynn Murphy, Hafeez Nathoo, Warren H. Finlay, Andrew R. Martin, *University of Alberta*

Modeling regional deposition of inhaled pharmaceutical aerosols in the respiratory tract provides useful information with which to assess dosing to targeted airways or lung regions. For single breath inhalers such as dry powder inhalers (DPIs) or pressurized metered-dose inhalers (pMDIs), the physics governing aerosol generation and deposition in the mouth and throat is complex, and difficult to capture with existing mathematical models. As such, for these inhalers it is common to estimate extrathoracic deposition experimentally, using idealized or realistic mouth-throat geometries. The size distribution of aerosol penetrating these geometries can then be measured, and used as input to models used to predict regional deposition through the lower airways of the lung.

Recently, predictions of regional deposition fractions have been coupled with models of dispersion, incorporating drug particle dissolution, mucociliary clearance, and absorption, in order to predict the duration of local and systemic exposure to inhaled drugs following aerosol delivery. Such predictions are valuable in assessing whether and for how long therapeutic drug concentrations are achieved in targeted lung regions, and in comparing relative exposures between alternative devices or formulations used to administer the same drug.

In the present work, we examined local and systemic drug concentrations over time following inhalation of budesonide from three different commercial DPIs. Extrathoracic deposition was measured *in vitro* using the Alberta Idealized Throat (AIT). Particle size distributions penetrating the AIT were measured using a Next Generation Impactor (NGI). The mass of drug captured by the AIT, and on each stage of the NGI, served as input to a regional deposition model used to predict deposited undissolved drug mass in each generation of the lung. Subsequent dissolution of drug in the airway surface liquid (ASL) was modeled as a Nernst-Brunner process. The ASL concentrations of dissolved drug in each airway generation, as well as systemic drug concentrations, were then predicted using a recently-developed compartmental disposition model, incorporating first-order rate constants to describe the competing processes of drug clearance and absorption from the lungs.

Predictions of local and systemic budesonide exposure will be presented and compared for the three DPIs studied. In addition, predicted concentrations of dissolved drug in the ASL will be discussed in relation to *in vitro* and pharmacokinetic metrics currently used to evaluate equivalency between inhalers.

4MD.7

Protein Aggregation Kinetics by Electrospray Differential Mobility Analysis. KALEB DUELGE, Vince Hackley, Michael Zachariah, *University of Maryland, College Park*

Protein aggregation is an important concern in protein therapeutics, resulting in adverse immunological response in patients. New therapeutics seeking FDA approval require some form of an induced aggregation study to indicate the stability of the formulation. Techniques to investigate aggregation include: fluorescence, analytical ultracentrifugation and light scattering with or without an initial separation step. Size exclusion chromatography and field flow fractionation separate the protein particles by size in solution and then detect the particles using light absorbance or scattering. These techniques allow for the calculation of aggregation kinetics by monitoring the loss of the protein monomer with time. We present results on the use of Electrospray Differential Mobility Analysis (ES-DMA) as an alternative means to study protein aggregation. ES-DMA is used to determine the temporal distribution of monomer, dimer and higher aggregates. These results are used to determine rate laws and rate constants under various thermal and buffer conditions. Comparison to more traditional methods will be examined.

4MD.8

Characterization of the Aerosol Flow, Sampling and Deposition in a Nose Only Exposure Chamber. FRANCESCO LUCCI, Wei Teck Tan, Subash Krishnan, Julia Hoeng, Patrick Vanscheeuwijck, Rudolph Jaeger, Arkadiusz Kuczaj, *Philip Morris International R&D*

For in vivo drug delivery or toxicological assessment, a variety of inhalation exposure chambers may be employed. In particular, rodent exposure in mice requires efficient and targeted exposure systems. The Nose Only Exposure Chamber (NOEC) produced by CH Technologies (USA) meets this need and simultaneously conveys aerosols to separated breathing ports. This feature limits other non-respiratory aerosol absorption paths that may complicate biological response analyses and it also minimizes the amount of test aerosol that is required for the exposure.

Any exposure system introduces a certain variability in the aerosol exposure caused either by the system design and functioning principles and/or limited influence to control behavior of the rodents. In our tailored NOEC system, the aerosol mixture flows vertically downward through an inner plenum and the aerosol is distributed horizontally through 60 exposure ports. These are staggered at 15 degree offsets between 5 adjoining tiers of 12 ports each. Ports are loaded with air tight glass tubes to separately host and position the mice. The aerosol is exhausted through an outer plenum peripheral to the inner plenum. A uniform aerosol delivery between all ports is desired for reliable performance of the exposure studies. The aim of the present analysis is to investigate aerosol flow characteristics in the NOEC system and estimate any potential size-dependent (> 1 mum) aerosol sampling non-uniformities at the mouse port. Such insight generally should lead to better understanding of the operating conditions during exposure and further optimization of the system.

For the investigations we have employed experimental and computational techniques. In particular, operating flow conditions and user-requirements concerning aerosol measurement devices make the acquisition of the experimental data very challenging. The novelty of our approach is the application of our recently developed Eulerian Computational Fluid Dynamics solver (AeroSolved: www.aerosolved.com) designed to simulate polydisperse multi-species aerosol transport and deposition. The aerosol equations include drag, gravitational and Brownian diffusion forces. We investigated aerosol transport and sampling through the main components of the system under actual operating conditions, obtaining unique verification data. Available experimental data concerning the flow were used to verify the computed results.

Computational results show that under operating condition, the central jet delivering the aerosol to the inner plenum produces a recirculation zone between the middle and the upper part of the plenum. The resulting pressure variations will cause a maximum flow variability of 20% at the ports, a result consistent with the acquired experimental data. Flow uniformity inside the plenum can be controlled by the adjustment of the aerosol delivery inlet diameter. Assuming operational flow rate at the port of and realistic in the average value inhalation flow rate to the closed by the mouse nose exposure tube, we have identified a small (<1%) preferential aerosol flux sampling to the nose port due to the aerosol drift from the flow streamlines near to the port. Detailed computational investigations will be presented along with the experimental verification of the system functioning for various aerosol flows.

4MD.9

Method for the Production of "Universal" Inhalation Powders for Dry Powder Inhalers. Janne Raula, DAVID BROWN, Esko Kauppinen, *Teicos Pharma*

Teicos Pharma has developed a unique inhalation drug formulation technology (trade named "Particle Stream Technology") which allows the production of highly flowable and dispersible inhalation powders (trade named "ProFlow Powder") from virtually any pharmaceutical agent and at low cost. This technology enables the production of highly efficient and fast acting inhalable "carrier free" formulations of wide range of active pharmaceutical ingredients (APIs), be they water soluable or insoluable, for pulmonary or systemic disease. The formulation also provides patients a painless and effective dosing procedure which avoids the side effects of traditional carrier containing inhalation formulations.

Carrier free formulations have been demonstrated to have a up to 99% API, compared to 1-2% API in traditional milled powders, Fine Particle Fractions (FPFs) above 55% compared to 10-15% in traditional milled powders and emitted doses of over 20x traditional milled formulations. In combination formulations including lactose carrier particles, we have achieved FPFs of greater than 90%. Emited doses have been demonstrated to be virtually independent of inhalation flow rate in the normal human inhalation range of 22 to 55 LPM. In-vitro tests have demonstrated safe biocompatablity.

4MD.10

Investigation of Single Particle Frictional Electrification with Polymer Plate. JIAWEI HU, Cai Liang, Lunbo Duan, Xiaoping Chen, Daoyin Liu, Changsui Zhao, *School of Energy and Environment, Southeast University*

In Dry Power Inhalers, the small drug particulates are always highly charged due to continuously contact with the device and other particles. The accumulation of static charges on drug particles may lead to particle- device adhesion which significantly affects drug delivery, drug disposal, and dosage in DPIs. In order to explore the mechanism of electrostatic charging in DPIs, a simplifying approach by investigating the triboelectrification of a single particle sliding on a polymer plate has been conducted in this work. To obtain the accuracy triboelectric charge due to sliding, the initial charge on the particle before sliding and the final charge after the particle separate from the plate were measured with two Faraday Cups. The results indicated that the final charge of the particle was found to be linear with the initial charge for a short sliding distance, whereas the experimental data became scattered for a long sliding length. The influences of the sliding length and normal load on the triboelectric charge density were analyzed by considering the contact area. Furthermore, the triboelectric charge density was able to be fundamentally described as a function of the sliding contact area and the real contact area.

4MD.11

Patient Specific Deposition Enhancement of Nasal Sprays in Ct-Derived Human Nasal Replicas. Landon Holbrook, ALYSSA BURKE, Saikat Basu, Elizabeth Monaghan, Julia Kimbell, William Bennett, *University of North Carolina at Chapel Hill*

A patient specific nozzle positioning device (NPD) was developed to enhance delivery of a nasal spray in an individualized nasal model of a patient post functional endoscopic sinus surgery (FESS). Preliminary computational fluid dynamics (CFD) simulations were used to determine administration angles for improved delivery to the maxillary sinus. Penetration depth past the nasal valve was established as a metric to assess improvement compared to standard of care (SOC) use as specified by package insert instructions.

Methods: De-identified sinus CT scans were used to digitally reconstruct the nasal cavity of a patient before and after FESS. Hollow models of the nasal cavity including external nares were 3D-printed in flexible and rigid parts to allow for nostril distension due to the insertion of a nasal spray bottle. The angle of administration was fixed1) according to SOC instructions or 2) for the NPD based on CFD simulation on the post-FESS model results. The NPD was retrofitted for testing on the pre-FESS model without CFD simulations. The SOC use condition was tilting the head at 22.5 degrees forward with an upright bottle inserted to a depth of one centimeter. Steady inspiratory airflow at a flow rate derived from subject weight was drawn through the model during administration of a nasal spray (one spray in left nostril) spiked with the radioactive tracer Tc99m. Radio-aerosol deposition was assessed using a 2D gamma camera. Images of the models in the coronal plane were used to quantify sinus deposition, while images in the sagittal plane were used for penetration measures. Four replicate experiments were conducted to determine the mean and standard deviation (SD) of deposition. Coefficient of variation (CoV) is used to estimate consistency between experiments and is determined by dividing the SD of the deposition by the calculated mean.

Results: Preliminary results for a single subject showed that the mean (SD) fraction of sprayed drug depositing posterior to the nasal valve was 8.0 (2.7) % of the total dose in the pre-FESS model and 11.4 (2.3) % of the total dose in the post-FESS model using SOC administration. Administration of the nasal spray with the NPD produced a mean (SD) fraction of posterior deposition of 12.7 (5.2) % in the pre-FESS model and 15.8 (1.4) % in the post-FESS model. The CoV was 20.4% using the SOC administration and 8.8% using the NPD in the post-FESS model. However, the CoV was 34.2% using the SOC administration and 41.1% using the NPD in the pre-FESS model.

Conclusions: SOC administration of a nasal spray product was measured using gamma scintigraphy and increased 42% when comparing a pre-FESS surgery model to a post-FESS model. Use of the NPD provided a 39.0% increase in deposition posterior to the nasal valve in the post-FESS model. Variability was reduced for the post-FESS model, likely because the NPD was a better fit for this model. Additional subject models are being tested to determine if the NPD will consistently reduce the variability in administered dose. While the novel positioning device coupled with surgery improved delivery of a nasal spray past the nasal valve from 8.0% to 15.8%., there is a remaining 84.2% of the drug depositing prior to the nasal valve that is not expected to provide any therapeutic effect. Supported by NIH HL122154.

4MS.1

MOFs-based Hybrid Nanocomposites for Efficient Gas Capture and Conversion: A Charge Transfer Study. Xiang He, WEI-NING WANG, *Virginia Commonwealth University*

Metal organic frameworks (MOFs) are an exciting class of highly porous polymer crystals with superior surface areas, tunable porosities, and rich functionality, enabling them for a variety of applications in energy and environmental sectors. We have developed aerosol-based synthetic strategies to integrate MOFs with semiconductors to form hybrid nanocomposites for various environmental applications, such as CO_2 adsorption and photoreduction. With increased charge carrier density and efficient CO_2 activation, the hybrid ternary nanocomposite exhibits a high CO_2 conversion efficiency and preferential formation of CH_4. Systematic measurements by using gas chromatography, photoluminescence spectroscopy, X-ray photoelectron spectroscopy, and time-resolved in-situ diffuse reflectance infrared Fourier transform spectroscopy reveal that the semiconductor heterojunction and the coordinatively unsaturated copper sites within the hybrid nanostructure are attributable to the performance enhancements.

4MS.2

Fabrication of Iron Oxide Nanoparticles Deposited on Crumpled Graphene for Supercapacitor Applications.

CHONGMIN LEE, Sun Kyung Kim, Ji-Hyuk Choi, Hankwon Chang, Hee Dong Jang, *Korea University of Science and Technology*

Supercapacitors have attracted considerable attention in recent years because they are able to provide high power density, fast charge process, long cycle life, and low maintenance cost. The performance of supercapacitors is largely determined by the properties of the electrode materials. So far, there are mainly three kinds of electrode materials: carbonaceous materials, transition metal oxides and conducting polymer materials. Among them, transition metal oxides have been widely investigated as pseudocapacitor electrode materials owing to their potentially high specific capacitance. Recently, iron oxides have emerged as alternative electrode materials for supercapacitors because they have advantages of low cost, natural abundance, and environmental friendliness. Graphene loaded with hematite (Fe_2O_3) or magnetite (Fe_3O_4) exhibited enhanced specific capacitance as well as a high energy density. In this study, we present three-dimensional (3D) crumpled graphene (CGR) decorated with Fe_2O_3 and Fe_3O_4 nanoparticles to determine which one can exhibit higher electrochemical performance of supercapacitors. The 3D CGR-Fe_2O_3 and 3D CGR-Fe_3O_4 composites were synthesized in different gas atmospheres from a colloidal mixture of GO and from iron (III) chloride hexahydrate ($FeCl_3 \cdot 6H_2O$), respectively, via one step aerosol spray pyrolysis. Sizes of both iron oxides nanoparticles were ranged from 5 to 10 nm when loaded onto 500 nm CGR. The electrochemical properties of the 3D CGR-Fe_2O_3 and 3D CGR-Fe_3O_4 composites were examined to compare the electrochemical performance of both composite electrodes. The 3D CGR-Fe_3O_4 composite electrode had 16% higher values of capacitance and electrical conductivity than those of the 3D CGR-Fe_2O_3 composite electrode.

4MS.3

Femtoliter Droplet Cloud Evaporation in an Aerosol Reactor. Yuliya Khodyko, SERGEY FISENKO, Wei-Ning Wang, *Luikov Institute of Heat and Mass Transfer*

Results of experimental investigations and simulations of the evaporation of femtoliter water droplet cloud in a laminar flow aerosol reactor are presented. Evaporation of the droplets under atmospheric (continuum regime) and low pressure environments (free molecular regime) are considered. Evaporation of droplets of aqueous solution creates a supersaturated solution inside and it decays via formation of nanoparticles. It was shown that even for temperature wall above 1000 K and reactor length around 1 m, the droplet temperature is significantly decreased by several hundred K. In free molecular regime, the droplet evaporation is running at practically constant temperature. For evaporation in continuum regime, the evaporation rate is strongly depend on droplet radii. Micron-sized droplet practically evaporated during a several hundredths of the second. The larger droplet radius the smaller the solution supersaturation inside it. It is shown that evaporation rate is substantially lower if the number density of droplets increases. The similarity criteria of evaporation and related heat and mass transfer are developed.

4MS.4

Engineered Chitosan and Aerosol Delivery Improve Plant Protection and Reduce Agrochemical Stress on Environment.

Rampura Vishwanath Kumaraswamy, Sarita Kumari, Ram Chandra Choudhary, Shyam Sundar Sahrma, Ajay Pal, RAMESH RALIYA, Pratim Biswas, Vinod Saharan, *Maharana Pratap University of Agriculture and Technology, IN*

Intensive use of agrochemicals for crop protection contributes to environmental pollution, in particular water, food and soil. Moreover, over the period of time, pathogenic microbes develop resistance against such chemical thus effectiveness become lower. Therefore, it is required either to develop the effective antimicrobial agent that can release slowly and in a controlled fashion or resistance in the plants against the pathogenic organism. In the present investigation, we synthesized chitosan (diameter between 200 and 370 nm) decorated with inorganic (i.e Cu) or organic (i.e. salicylic acid) substances. We characterized the engineered chitosan for its stability and physicochemical properties. Further, the chitosan formulation tested on corn and tomato. The formulation was delivered to these plants by a foliar aerosol spray. Resultant we observed that the functionalized chitosan nanoparticles boost the plant resistance by altering reactive oxygen species or mobilizing reserve food. The predictable role of engineered chitosan in plants might be in achieving sustainable plant growth through boosting the intrinsic potential of plants. In-spite of the fact that engineered chitosan abode immense biological activities in plants, these materials have not yet been widely adopted in agriculture due to poor understanding of its bioactivity and modes of action towards pathogenic microbes and in plant protection and growth. Our findings not only highlighted in-depth, various engineered chitosan formulation which has been tested for plant growth and protection mainly against fungi, bacteria and virus but also explained their modes of action.

4MS.5

Detonation Graphene Production Scale Up. JUSTIN WRIGHT, Arjun Nepal, Stefan Bossmann, Christopher Sorensen, *Kansas State University*

We describe our efforts to scale up the production of graphene powders produced by the detonation synthesis method. Historically, the detonation synthesis method began with a tedious gas fill-up phase, and ended with a long clean-out phase. We added electronic flow-meters to speed up the fill-up phase, and tested how fill-up time impacts the quality and yield of the final sample. We also ran tests on the chamber size to prove that the same sample quality and fractional yield was obtained. Finally, to improve the clean-out phase, a system to withdraw the sample after detonation was developed and tested. With all of these parameters, we push to achieve production of 1kg of detonation graphene per day.

4MS.6

The Study of the Role of Morphology and Functional Groups of Crumpled Graphene-based Materials to Determine their Specificity Towards Volatile Organic Compounds in Room-temperature Gas Sensing. KELSEY HADDAD, Siyuan An, Ahmed A. Abokifa, Barani Raman, Fortner John, Pratim Biswas, *Washington University in St. Louis*

Chemiresistive gas sensors, introduced in 1962, detect gases through changes in the electrical resistance of a semiconducting material as a function of the surrounding atmosphere. These gas sensors are already prevalent in areas such as environmental monitoring, domestic safety, and industrial processing for monitoring of toxic gases, including nitrogen dioxide, carbon monoxide, ammonia, and nitric oxide, among others. Graphene-based materials show room temperature gas sensing properties, and the functionalization of graphene is an easy approach to modulating sensitivity; nevertheless, their response suffers from long recovery times. A thorough understanding of the interaction between the sensing material and the analyte of interest is an important step in the practical application of these highly tunable materials for selective gas sensing. Crumpled graphene oxide (CGO), with a minimal tendency towards aggregation while still maintaining the high specific surface area and exceptional electronic properties of flat sheets, offers a potential solution for the integration of reduced graphene oxide into scalable and reproducible chemiresistive sensors.[1-3] Crumpled graphene, in contrast to 2D flat analogs, has not been studied for gas sensing applications. Moreover, the crumpled ridges of the CGO sheets can be considered as line defects, which should enhance adsorption. To date, the majority of studies for graphene and graphene oxide have focused on environmental gases, with no study systematically looking at the role of functional groups or nanostructured materials on sensing volatile organic compounds (VOCs). The diverse responses seen across different classes of VOCs (apolar, monopolar, and bipolar) will be explored to give insight into the interaction mechanisms of graphene oxide and CGO. The role of morphology and functionalization on the sensing response and mechanism of carbon-based materials was systematically explored by crumpling and reducing graphene oxide sheets. Ultimately, the insights gained by correlating the sensor response to analyte and material properties can aid in the construction of an array focused on sensing specific VOC profiles.

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4MS.7

Synthesis of Nanoparticle-embedded Composite Films by Plasma-enhanced CVD Process Using Gaseous and Particulate Raw Materials. MANABU SHIMADA, Masaru Kubo, Yuki Shigematsu, Izumo Shimada, *Hiroshima University*

Nanocomposite films consisting of different species are attracting interest, because of the integrated or synergistic properties of the species. Among these, thin films with embedded nanoparticles are promising materials for many applications. The properties of the embedded nanoparticles, such as size and quantity, should sufficiently be controlled in order for desired properties to emerge. One of the beneficial ways to control the properties is to use pre-formed nanoparticles. In this study, nanocomposite films in which silicon dioxide (SiO_2) nanoparticles and carbon nanotubes (CNTs) are embedded in titanium dioxide (TiO_2) matrix are synthesized by a combination of a spray-drying aerosolization technique and plasma-enhanced chemical vapor deposition (PECVD).

TiO_2 matrix is synthesized by feeding titanium tetraisopropoxide (TTIP) vapor in a microwave plasma field. An SiO_2 nanoparticle or CNT suspension is sprayed into the plasma field simultaneously, in which the sprayed droplets are electrically charged and broken-up by Coulomb explosion to generate an aerosol with well-dispersed nanoparticles. This simultaneous feeding of the vapor and nanoparticle aerosol produces the nanocomposite films on silicon and quartz-glass substrates by PECVD. The concentration and size of the nanoparticles in the suspension influenced the morphology and inner structure of the films. Quantitative evaluation of the surface roughness of the films reveals the roughness formation due to the embedded nanoparticles. The photocatalytic activities of the films are found to be enhanced, as compared to that of a TiO_2 film, probably because of the increase in the surface area of the films due to the roughness.

4MS.8

Polymer and Metal Oxides Coating of Multiwalled Carbon Nanotubes by Spray-Assisted Plasma-Enhanced Chemical Vapor Deposition.

LAKSHMIPURA RAMACHANDRAIAH HEMANTH, Keita Nishihara, Masaru Kubo, Manabu Shimada, K. Kusdianto, *Hiroshima University*

Carbon nanotubes have wide applications in every sector due to the tuneable surface property. The low thermal conductivity and surface oxidization of carbon nanotubes limit their applications. To overcome these problems, surface coating is preferred. The coating is performed by physical, chemical as well as by mechanical methods. The present work details about the coatings on surface of carbon nanotubes by polymers and metal oxides by spray-assisted plasma-enhanced chemical vapor deposition (PECVD). Two different streams containing aerosolized multiwalled carbon nanotubes and vaporized methyl methacrylate or metal alkoxides is sprayed simultaneously into plasma; to develop coated carbon nanotubes on a silica substrate by PECVD. The stoichiometry of polymeric materials and metal oxides with focus on retention of desired nanostructures is evaluated. The effects of process conditions such as pre-treatment of nanotubes, carrier gas, flow parameters are analysed. Developed material is characterized basically by X-ray diffractometer, scanning electron microscopy, transmission electron microscopy, FTIR and by Raman spectroscopy. Coated porous polymeric materials on nanotubes surface with thickness of 100-400 nm are obtained under the controlled reaction conditions with acid pre-treatment. Surface morphology of obtained material reveals un-destructed carbon nanotubes with uniform coating of polymer and metal oxides.

4MS.9

Effect of Loading Concentration on the Photocatalytic Activity of Ag-TiO2 Nanocomposite Films Fabricated by One-Step Gas-Phase Deposition. DIANPING JIANG, K. Kusdianto, Masaru Kubo, Manabu Shimada, *Hiroshima University*

It is well known that adding Ag nanoparticles in TiO_2 matrix enhances the photocatalytic performances. It is mainly caused by reducing the electron-hole recombination in photocatalytic reaction due to metal-semiconductor junction. For preparation of Ag-TiO_2 nanocomposites, varieties of routes have been approached which can be categorized as liquid and gas methods, etc. However, fabrication methods included in the liquid methods have disadvantages of having a large number of processing steps, using high temperatures under vacuum conditions, and concern on impurities involved. In this study, Ag-TiO_2 nanocomposite thin films on silicon substrate with different Ag concentrations were synthesized in gas phase by a combination of plasma-enhanced chemical vapor deposition (PECVD) and physical vapor deposition (PVD). The nanocomposite films with different Ag concentrations ranging from 0 to 12.7 wt% were prepared by changing the amount of Ag vapor in the PVD system. It is obviously observed that the crystalline phase, crystallite size, and particle size of the fabricated Ag-TiO_2 nanocomposite films after annealing at 500 °C were affected by the concentration of Ag nanoparticles. The existence of very small Ag nanoparticles (~4 nm) in the films was also confirmed by transmission electron microscopy. Photocatalytic activity evaluated by measuring the degradation of methylene blue aqueous solution under UV light irradiation exhibited that a film with Ag nanoparticle concentration of 5.3 wt% showed the highest photocatalytic performance. This work will be significant not only in the preparation of Ag-TiO_2 nanocomposite films but also in the preparation of metal-semiconductor nanocomposite films which has wide potential applications in photocatalysis, solar energy conversion, antibacterial application, chemical sensors, and so on.

4MS.10

Generation of Iron Oxide Nanoparticles for Follow-up Exposure Studies by MOCVD. PAVEL MORAVEC, Jaroslav Schwarz, Petr Vodička, Jaroslav Kupčík, Jaroslav Švehla, *Institute of Chemical Process Fundamentals of the CAS, v.v.i*

Iron oxide nanoparticles (NPs) are industrially produced and commercially available and they are also frequently emitted into the environment by iron making plants. In the human body, iron is maintained at homeostatic fairly low level. However, freshly generated iron oxide NPs cause febrile and inflammatory response known as metal fume fever, but the potential in vivo consequences of inhalation of iron oxide NPs from the atmosphere has not yet been investigated. In this study we tested a method of long lasting generation of iron oxide NPs by pyrolysis and oxidation of ironIII acetylacetonate (FeAA3).

Experiments were performed in an externally heated work tube with i.d. 25 mm and 1 m long heated zone. A stream of nitrogen carrier gas, saturated by precursor vapours in a saturator (Q_S), was fed into the reactor, where it was mixed either with a stream of nitrogen (pyrolysis) or a mixture of nitrogen and air (oxidation). A stream of NPs laden gas (Q_R) was diluted in the outlet part of the work tube by a diluting stream (Q_{Dil}) of nitrogen (pyrolysis) or air (oxidation). The particle production was studied in dependence on reactor (T_R) and saturator temperature (T_S), and on flowrates Q_S, Q_R and Q_{Dil}, and NPs production was monitored using SMPS (TSI model 3936L75). Samples for NPs characterization were deposited onto TEM grids, using a nanometer aerosol sampler (TSI model 3089) and on cellulose, quartz, and Sterlitech Ag filters. The particle characteristics were studied using HRTEM (*JEOL 3010*), energy dispersive spectroscopy (*INCA/Oxford* connected to *JEOL 3010*), selected area electron diffraction (*JEOL 3010*), inductively coupled plasma – optical emission spectrometry (*Agilent 4200 MP-AES*), elemental and organic carbon analysis (EC/OC, Model 4, Sunset Laboratory) and X-ray diffraction (*Bruker D8 Discover diffractometer*).

Two experimental campaigns in total duration 100 and 80 hours were performed. The NPs production was studied in the range of T_R: 500-800 °C, T_S: 134-141 °C, Q_R: 1400-1500 cm^3/min, Q_S: 120-200 cm^3/min and Q_{Dil}: 1600-1700 cm^3/min. Results have shown that NPs generation by oxidation of FeAA3 at T_R 700 or 800 °C suits for long term inhalation exposure experiments. The generation provides NPs production rate sufficiently high (up to 2400 µg/m^3, i.e. 7.7 µg/min) and can be further increased by an increase of T_S or/and Q_S, and it is stable at steady state conditions for sufficiently long time. Primary particle size is typically between 10-20 nm, the content of Fe varies from 58.7 to 59.6 wt. %, which corresponds to 84.0 – 84.7 wt. % of Fe_2O_3. NPs are free of EC and contain only 3.6 – 5.2 wt. % of OC. Both XRD and SAED method identified cubic Fe_2O_3 crystalline phase, Pdf 32-0469. On the other hand, NPs generation by pyrolysis does not seem to be perspective method for exposure experiments due to poorly defined characteristics of NPs. They contain a lot of EC (32.2 – 37.7 wt. %), the content of Fe varies between 22 and 52 wt. % and because the NPs are amorphous, it is very difficult to identify the form of Fe in NPs.

This work was supported by the Czech Science Foundation under grant P503/12/G147. XRD analyses were performed by Mgr. Petr Mikysek, Geological Institute of the CAS, and EC/OC analyses by Mgr. Věra Procházková, Institute of Chemical Process Fundamentals of the CAS.

4MS.11

Aerosol-assisted Synthesis of Materials for Application in Photovoltaics – TiO2 + Perovskite Layers. ROBIN WHEELUS, Shalinee Kavadiya, Pratim Biswas, *Washington University in St. Louis*

Perovskite solar cells' rapidly increasing power conversion efficiency and cheap cost of production have captured the attention of researchers world-wide and are fundamental reasons why these cells have become one of the fastest growing possibilities for energy production. As mentioned in previous abstracts, however, they face major challenges with stability, particularly in humid conditions. Electro-spray has been developed as a two-step method for perovskite layer formation, allowing for cell fabrication under ambient conditions with both increased efficiency over spin coated cells and relative stability over 5.5 months[1]. The technique is successful largely because of the smooth perovskite surface it produces, which mitigates the perovskite-water interaction. However, electro-spray's effectiveness over a rough surface morphology, like the one obtained from aerosol chemical vapor deposition, has not previously been investigated. This research aims to address questions as to how the electron transport layer (ETL) and perovskite layers interact when the two are deposited using ACVD and electro-spray respectively. Ideally, we aim for a perovskite layer that comes into contact with the entire surface of the electron transport layer in order to take advantage of both the shorter electron pathways from electrons separating at the base of the columns and the increased surface area from the modified morphology. Furthermore, in order to benefit from electrospray's primary advantage, we also want to maintain a smooth perovskite surface above the ETL. We will compare cross-sectional SEM images and power conversion efficiencies for spin-coated and electro-spray deposited perovskite cells with columnar electron transport layers in order to understand and improve the compatibility of these two aerosol techniques in this application.

Reference
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4MS.12

Attachment Behavior and Aggregation Kinetics of Aerosol Synthesized Oxide Nanomaterials in Water. RAMESH RALIYA, Nathan Reed, Kwon Paul, Tiana Stussie, Patchaya Tobarameekul, Deep Hathi, Patcharin Worathanakul, Samuel Achilefu, Monica Shokeen, Pratim Biswas, *Washington University in St. Louis*

Oxide nanomaterials such as TiO2, Fe2O3, SiO2 and ZnO are manufactured at industrial scale for various applications such as paint, food and cosmetics. Recently, these nanomaterials are being explored for advanced biomedical applications including but not limited to cancer therapeutics, deep-tissue imaging and drug delivery. However, at nanoscale (between 1 and 100 nm at least at one dimension) these particles tend to agglomerate/aggregate very rapidly in the biologically compatible or FDA approved solvents for drug formulation. Because of the aggregation/agglomeration, it is very hard to harness the desired potential of the surface area to volume size phenomenon at the nanoscale[a,b]. In the present study, we investigate mechanistic of oxide nanomaterials aggregation or agglomeration behavior and elucidate the relationship between water chemistry and nanoparticle surface. We compared TiO2, Fe2O3, SiO2 and ZnO nanoparticles synthesized from two different methods, namely- flame/furnace aerosol and sol-gel. Particle stability and aggregation behavior were studied using time-resolved – dynamic light scattering (TR-DLS), and electron microscopy. Surface chemistry of the nanoparticles was characterized by electron microscopy and photon correlation spectroscopy. The data obtained from TR-DLS were used to calculate attachment efficiency of two particles. In summary, the study mechanistically reveals the particles behavior in the solvent and offer solvents conditions (pH, Ionic strength, zeta potential, concentration and physical force) to keep the oxide particles in their monodisperse state independent of the synthesis procedure.

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4MS.13

Electrospray Deposition as a Tool for Processing Energetic Polymer Composites. Haiyang Wang, MICHAEL ZACHARIAH, *University of Maryland, College Park*

Electrospray is shown as a tool in the preparation of nanoenergetic based composites with a variety of morphologies ranging from fibers, microparticles composites and thin films, by varying precursor concentrations, binder content, nanoparticle loading and flight time. Examples will be described including the formation of thermite based nanofiber mats with a nitrocellulose composite energetic binder to create a new class of energetic 1-D nanocomposite. Employing electrospray as a means to create a gel within a droplet by evaporation induced rapid aggregation, enables us to generate microparticles of nano-aluminum and oxidizer nanoparticles. We find that the average size of the microparticles can be systematically changed from 2 µm to 16 µm. Finally by preventing drop evaporation the electrospray deposition method is employed to create high loadings of aluminum nanoparticles (Al-NPs) in polyvinylidene fluoride (PVDF) reactive composite films. The deposited films containing up to 50 wt % Al are found to be crack free and mechanically flexible.

In all cases the combustion performance was evaluated by a variety of metrics.

4MS.14

Synthesis of CuO/WO3 and Pt/WO3 Nanocatalysts via Flame-Assisted Spray Pyrolysis and Their Photocatalytic Activity. TOMOYUKI HIRANO, Ogi Takashi, Kikuo Okuyama, *Hiroshima University*

Tungsten oxide (WO_3) has been regarded as visible-light-driven photocatalyst and many other potential applications. However, pure WO_3 shows very low photocatalytic performance under visible light irradiation. One of the promising method to solve this problem, addition of another metal in the WO_3 has attracted attention.

In this work, CuO/WO_3 and Pt/WO_3 nanocatalysts were successfully synthesized using a flame-assisted spray pyrolysis (FASP) method. FASP is an attractive process that enables us to control the particle size, crystal size, and morphology of prepared particles by controlling fuel and carrier gas flow rates, concentrations of precursor, and so on. The flame-made nanocatalysts have strong interconnection between WO_3 and co-catalysts, and they were effective for degrading of aqueous organic pollutant under visible light irradiation. The Pt/WO_3 nanocatalyst exhibited optimal photocatalytic performance with a low Pt concentration of 0.12 wt.%, which is much lower compared to the reported optimal concentrations using a photodeposition technique (0.5–1 wt.%). It is necessary to reduce the required Pt amount in the Pt/WO_3 photocatalysts for large-scale and practical applications.

The addition of CuO enhanced the photocatalytic activity of WO_3 for dye photodegradation under visible light irradiation. The morphology of WO_3 was changed from nanorods to cubic following the addition of CuO. The CuO/WO_3 composite with 0.33 wt.% CuO concentration exhibited the best photocatalytic activity. Furthermore, during a photodegradation test, the as-prepared particles were mechanically stable. Thus, the FASP method is a promising process for the production of a low cost WO_3-based photocatalyst.

4MS.15

Gas-phase Synthesis of Gallium Arsenide Quantum Dots through Hydrogen-assisted Spark Discharge and Its Application.

KIWOONG LEE, Dongjoon Lee, Mansoo Choi, *Seoul National University, Seoul, Korea*

Gallium Arsenide (GaAs) has been considered as one of the most prominent III-V semiconductors because of its extraordinary electronic and photonic properties, such as high electron mobility and direct band gap. Furthermore, because of its large Bohr radius and strong quantum confinement effect, there have been intense effort to synthesize GaAs nanocrystals (NCs) with diameter of under 20 nm. However, despite these advantages of GaAs NCs, there has been inherent difficulties of synthesizing GaAs NCs restricting its applications toward practical devices as well as overall exploration.

Recently, our group introduced hydrogen gas toward spark discharge between silicon (Si) electrodes and demonstrated that hydrogen gas enabled silicon (Si) nanocrystals to be highly pure and crystalline. (D. Lee et al, 2016) In this research, crystallization of Si nanoparticles was based on the scheme in which amorphous Si matrix become crystalline by hydrogen atom's insertion into and relaxation from Si bonds. (S. Srirman, 2002) However, unlike Si, GaAs NCs are hardly obtained by hydrogen-assisted spark discharge since spark discharge energy is not sufficient for the relaxation of hydrogen atoms from GaAs matrix. We identify the amorphous GaAs nanoparticles embedding hydrogen atoms in GaAs matrix via transmission electron microscopy (TEM) and Fourier transform infrared spectroscopy (FTIR). In order to extract these embedded hydrogen atoms and thus to crystallize GaAs nanoparticles, we add heating procedure. After generation of hydrogen-inserted GaAs nanoparticles via hydrogen-assisted spark discharge, these amorphous GaAs aerosols pass through tube furnace with temperature of 950ºC for the desorption of inserted hydrogen atoms. It is demonstrated that fabricated GaAs NCs exhibit high crystallinity through TEM and X-ray diffraction (XRD) measurements.

Additionally, we demonstrate that these GaAs NCs exhibit quantum confinement effects from photoluminescence measurement. We generate GaAs NCs with various size by varying the capacitance of spark discharge circuit from 0.5nF to 6nF, and observe that these GaAs NCs exhibit different photoluminescence peaks according to its size.

Even though there are several other methods of fabricating GaAs quantum dots (QDs) such as chemical synthesis, chemical vapor deposition (CVD), and molecular beam epitaxy (MBE), these methods possess inherent drawbacks, such as expensive installation, undesirable by-products, toxic materials and poor controllability. Since our aerosol-based technique is free from these obstacles, we look forward to our GaAs QDs to be utilized in various applications, such as solar cell, LED, and transistor. In addition, our fabricating GaAs QDs technique is expected to provide an additional degree of freedom in synthesizing various semiconductor quantum dots with high crystallinity.

This work was supported by Global Frontier R&D Program on Center for Multiscale Energy System by National Research Foundation (NRF) under the Ministry of Science, ICT and Future Planning, Korea (Grant no.2012M3A6A7054855).

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4MS.17

Production of Cauliflower-like Amphipathic Copolymer Nanoparticles using Aerosol-Photopolymerization. Masoom Shaban, Jalal Poostforooshan, ALFRED P. WEBER, *TU Clausthal*

Amphipathic copolymers consist of hydrophilic and hydrophobic monomer units have attracted great technological attention recently, owing to their unique properties and their ability to stabilize various interfaces in aqueous systems. However, producing these copolymers is still a great challenge in liquid phase due to different polarities of monomers. As a promising alternative to the conventional liquid methods, the polymer nanoparticles can be prepared by an aerosol-polymerization. This method can also avoid the requirement of surfactants and solvents, and produce directly solvent-free dry powders with a high purity and spherical morphology in a continuous process which is desirable in pharmaceutical applications.

The work presented here describes a continuous aerosol-photopolymerization to produce different kind of spherical polymer nanoparticles including polyacrylamide (PAM), polystyrene (PS) and hydrophobically modified polyacrylamide (HM-PAM) *[1]*. The experimental setup is a combination of an atomizer, a homemade flow-through photoreactor, and a collection filter. Initially, the monomer droplets consisting of dissolved photoinitiator were generated by the atomizer. Then, sprayed droplets were passed through the photoreactor, where the free radicals were generated upon UV irradiation within the average aerosol residence time of 30 s in the photoreactor. To control the aqueous solubility, size and morphology of the resulting HM-PAM copolymers, different styrene/acrylamide monomer concentrations were introduced into the system.

The textural properties of the obtained materials were characterized by TEM, SEM, and N2 adsorption-desorption isotherms. The results revealed that the copolymers and polyacrylamide have cauliflower-like morphologies, while polystyrene has a nearly smooth morphology. Moreover, chemical compositions of the obtained materials were investigated by several characterization techniques such as ^{1}H NMR, FT-IR, TGA and elemental analysis. ^{1}H NMR and elemental analysis of resulting copolymers microstructures displayed successful incorporation of styrene in the copolymer with a good agreement compared to initial ratios.

Importantly, the final particle size of resulting polymer nanoparticles could be controlled either by the concentration of solution or flow rate of the carrier gas. As an example, the nanospheres generated with the total initial concentration of 0.195 M and 0.468 M, lead to the average size of 103 nm and 199 nm, respectively.

[1] Shaban *et al.* , *Eur. Polym. J.*, **2016**, 83, 323–336.

4MS.18

Preparation of Nanospherical Mesoporous Carbon Nitride with High Surface Area using Aerosol Generated Mesoporous Silica and Its Application as a Photoinitiator for Aerosol-Photopolymerization.

JALAL POOSTFOROOSHAN, Masoom Shaban, Alfred P. Weber, *TU Clausthal*

The work presented here describes a continuous aerosol-based process to produce submicron spherical polymer particles using nanospherical mesoporous carbon nitride (NMCN) as a photoinitiator. In this regard, spherical raspberry-like silica particle was initially synthesized by spray drying of nanocolloidal silica, using polyvinylpyrrolidone (PVP) as a template, within the average aerosol residence time of 6 s in the tube furnace reactor. After removal of the PVP by calcination, spherical mesoporous silica (SMS) nanoparticle was obtained. Then, NMCN with a high surface area and pore volume has been synthesized via a nanocasting approach by using SMS as a hard template through a simple polymerization reaction between ethylenediamine and carbon tetrachloride as precursors *[1]*.

The textural properties and chemical compositions of the obtained materials were investigated by employing diverse characterization techniques such as scanning mobility particle sizer (SMPS), N_2 adsorption-desorption isotherms, transmission electron microscopy (TEM), scanning electron microscopy (SEM), Raman, small-angle X-ray scattering (SAXS), X-ray photoelectron spectra (XPS), FT-IR, wide-angle X-ray diffraction (XRD), thermogravimetric analyzer (TGA), and CHN analyses. The results revealed that the NMCN has a high nitrogen content (16.8 wt%) with a high surface area of ~718 m^2/g, a pore volume of 1.22 cm^3/g and a pore size of 23 nm.

In addition to experimental characterization, the optical properties of NMCN were studied theoretically by three-dimensional finite difference time-domain (FDTD) method. Experimental and simulation results confirm that the introduction of desired mesoporosity in the carbon nitride not only increases the surface area for accommodating active sites, but also improves the light absorption and consequently increases the generation rate of electron-hole pairs inside the NMCN.

Finally, NMCN nanoparticles exhibit excellent performance in photopolymerization of butyl acrylate monomer in the continuous aerosol-based process, within the average aerosol residence time of 90 s in the photoreactor. In this one-pot synthesis, NMCN nanoparticles acting not only as photoinitiators, but at the same time as fillers and templates.

The presented aerosol-photopolymerization process operates at room temperature and avoids the need for solvent and surfactant. More importantly, with this method, we could overcome the problem of producing composites of carbon nitride with hydrophobic polymers. Furthermore, we simulated the condition of NMCN nanoparticles during illumination in the gas phase process which can freely rotate. The results demonstrated that the hole density is almost equally distributed in the whole part of the NMCN nanoparticles, leading to efficient light harvesting and more-homogeneous photoreaction.

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4MS.19

Preparation of Core-Shell Nanoparticles by Aerosol-Polymerization Process. JALAL POOSTFOROOSHAN, Masoom Shaban, Alfred P. Weber, *TU Clausthal*

Core-shell nanoparticles, consisting of an inorganic scaffold and polymeric shell, have received considerable attention due to their promising applications. These nanoparticles have the potential to combine different properties of the core and shell into a single particle. Generally, polymer shells on the inorganic nanoparticles prevent particle-particle aggregation and offer excellent compatibility in a polymer matrix.

In this work, inorganic cores were initially generated by either spark discharge followed by the sintering furnace (spherical Ag nanoparticles) or nebulization of the respective suspension (SiO_2 nanoparticles). Then, the inorganic nanoparticle-laden nitrogen flow was bubbled through the saturator containing the glycidyl methacrylate (GMA) as organic monomer kept usually at 80 °C. In the subsequent cooling behind the saturator back to room temperature a supersaturation was achieved resulting in the condensation of GMA vapor on the surface of the inorganic nanoparticle. Subsequently, the monomer coating was chemically polymerized ‘‘in flight’’ to form a polymer shell by addition of ammonia vapor as an initiator within the average aerosol residence time of 2 min in the polymerization reactor *[1]*. Moreover, the effect of numerous parameters, including the GMA saturator temperature and properties of inorganic nanoparticles on the structure of polymeric shell and coating thickness and efficiency has been investigated.

The particle size distribution and morphology of the resulting core-shell nanoparticles have been studied via scanning mobility particle sizer (SMPS) and transmission electron microscope (TEM). Finally, the coating efficiency was determined by aerosol photoemission (APE) and the results showed that monomer and polymer coating efficiency were 99% and 60%, respectively.

Highlights of the presented aerosol-polymerization procedure are the continuous, fast, simple and requires few unit operations. Moreover, in contrast to conventional wet methods such as emulsion polymerization, this technique can produce highly pure surfactant-free polymer shells and allows for a direct collection of composite nanoparticles.

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4MS.20

Aerosol Gelation in a Buoyancy-Opposed Flame Reactor: Application to Material Synthesis. PAI LIU, Yang Wang, Jiaxi Fang, Pratim Biswas, Rajan K. Chakrabarty, *Washington University in St Louis*

Aerosol gels are a novel class of materials with potential to serve various energy and environmental applications. Synthesis of aerosol gel materials in gas-phase could be a cost-effective alternative to the conventional wet sol-gel process. Past studies have shown nanoparticle gelation occurring in a down-fired, buoyancy-opposed flame aerosol reactor (BO-FAR) as a viable technique for scalable production of gel materials. However, this gas-phase technique has yet to be proved capable of synthesizing gels with tunable material properties. In this work, we present the results of our experiments specifically aimed at controlling the primary particle properties of gels using a BO-FAR. We were able to optimize the operating temperature conditions of the BO-FAR between 1250 and 590 °C by adjusting the oxidizer dilution ratio. At these two extreme temperature conditions, we delivered Titanium tetraisopropoxide (precursor) to the BO-FAR for producing carbon-free titanium dioxide (TiO_2) gel particles. Our results show approximately tenfold increase in the primary particle size of the TiO_2 aerosol gel with the increase in the flame temperature. Pure rutlile and anatase phase TiO_2 were formed at the high and low temperature conditions, respectively. Our work demonstrates that non-carbonaceous aerosol gel materials can be synthesized through a rapid single-step gas-phase process with high purity and tunable material properties.

4MS.21

Highly Reproducible Large-Area Perovskite Solar Cells Fabricated with Megasonic Spray-Coating. MINCHEOL PARK, Woohyung Cho, Mansoo Choi, *Seoul National University*

The thin-film solar cells using organometal halide perovskite have been establishing rapid rise in efficiency as a highly promising photovoltaic device for solar energy conversion. State-of-the-art devices achieved power conversion efficiencies (PCEs) of 22.1 %; this value surpassing the record efficiencies of amorphous silicon and organic semiconductor PV. As development of perovskite solar cells (PSCs), there have been few reports of scalable film-coating techniques being applied to the deposition of large-sized perovskite films. It is apparent that the path towards commercialization of solution-processed perovskite solar cells requires the development of fabrication methods for linear coating techniques such as roll-to-roll or sheet-fed processing techniques. Large-scalable coating techniques such as aerosol spray, slot-die, inkjet printing, and blade coating show the capability to scalable coat perovskite thin films[1, 2].

Herein, we report a highly promising technique using aerosol coating method generated by megasonic nebulizer also known as megasonic spray coating (MSC). By adapting MSC, efficient and reproducible large-area planar perovskite solar cells (PSCs) were successfully developed. The coating based on mist precursor can be easily operated with low-temperature and antisolvent-free process under ambient conditions. And it can effectively control the volume of $CH_3NH_3PbI_3$ precursor solution and the reaction temperature, which affect the quality of perovskite harvester layers and the performance of perovskite solar cells remarkably. Under optimized condition, the power conversion efficiency (PCE) of devices reach 17.0 % with the average PCE of 16.4 %. The megasonic spray method is also used to fabricate large-area solar cells (1 cm^2) and a PCE of 14.2 % is obtained.

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4MS.22

The Formation of Sulfur Trioxide over V2O5/TiO2 Catalyst in SCR of NOx with NH3. YURAN LI, Bin Wang, Jin Xiong, Tingyu Zhu, Shuai Zhang, *Institute of Process Eng., Chinese Academy of Sciences*

The oxidation of sulfur dioxide (SO2) to sulfur trioxide (SO3) is undesirable during the selective catalytic reduction (SCR) of nitrogen oxides (NOx) found in the flue gas of power plants. Sulfur trioxide has a toxicity over ten times than that of SO2 and is highly corrosive, a resource of aerosol. The objectives of this research are to establish the fundamental kinetics and mechanism of SO2 oxidation over supported V2O5/TiO2 catalyst and establish sulfur balance, then, use these insights to propose a basic theory for collaboratively controlling SO3 emissions. A series of supported V2O5/TiO2 catalysts were prepared with various V2O5 contents: 0.5%, 1%, 1.5%, 3%, 4% and 5%. Raman spectroscopy is used to determine the coordination of surface species. Isolated vanadia species were dispersed on the TiO2 surface as Ti-O-V bonds at VOx coverage below the monolayer. Sulfur dioxide temperature-programmed desorption and in situ diffuse reflectance infrared Fourier transform spectroscopy were conducted to study the interaction between SO2 and V2O5/TiO2. It was found that Ti-O-V was demonstrated to play a critical role in the SO2 adsorption and oxidation. A possible reaction mechanism of SO2 oxidation over V2O5/TiO2 catalyst was established in this study. The turnover frequency for SO2 oxidation was very low, approximately 10-5 s-1 at 320℃. Over the range of conditions studied, the rate of SO2 oxidation is zero-order in oxygen and first-order in SO2, and the apparent activation energies for SO2 oxidation was obtained. The decrease of SO2, the gaseous SO3 and the sulfate deposited on catalyst surface were to be quantified by Fourier transform infrared spectrometer (FTIR), PENTOL SO3 analyzer and ion chromatography (IC), respectively. Then, the sulfur balance was established.

4MS.23

Particle Size Distribution and Concentration of Gold Colloidal Nanoparticles. JAESEOK KIM, Min Jeong Kwak, *Korea Research Institute of Standards and Science*

Nanoparticles controlled by size and shape in water are significant to investigate toxicity of nanoparticles. In this present work, we develop well-controlled gold nanoparticles having 30 and 80 nm. The gold nanoparticles were characterized with respect to their shape and size by transmission electron microscopy (TEM) and scanning electron microscope (SEM). Particle size distribution in gold colloidal nanoparticles was determined by the electrospray scanning mobility particle sizer (ES-SMPS) and we compared it with an average particles size measured from dynamic light scattering (DLS). The geometric mean diameter (GMD) obtained by ES-SMPS was in good agreement compared to DLS results.

4MS.24

Constitution Analysis of CNT Aerogel and Its Thermal Property Modification and Characterization. ZHANG XIAO, Adam M Boies, *University of Cambridge*

Due to the outstanding properties of individual carbon nanotube (CNT), their corresponding assemblies, CNT aerogel and corresponding mat have been research hotspots for years as advanced electrical and thermal material. By using the one-step continuous growth technique (floating-catalyst chemical vapor deposition, FCCVD) and continuous collection method, scale up synthesis of CNT aerogel has realized and shown a bright future of CNT aerogel applications.

However, the degradation of properties when individual CNTs were used to form assemblies (including CNT aerogel) have been repeatedly shown in reported and our experiment results.

The large discrepancy between bulk thermal properties and individual CNTs motivated high-fidelity characterizations of CNT constitution after aerogelation, especially individual CNTs' length in aerogel, due to its significant effect on CNT-CNT overlapping length and junctions number in aerogel, and then heat conduction pathway in CNT aerogel.

This presentation will firstly report an ex situ characterization of individual CNTs from the CNT aerogel. De-aerogelation was realized by extracting and isolation of individual CNTs from intertwining CNT aerogel. With dynamic light scattering (DLS) analysis, scanning and transmission electron microscope (SEM and TEM), atomic force microscopy (AFM), UV-Vis-NIR absorption spectroscopy and Photoluminescence and Raman analysis, the constitution unit of CNT aerogel have been characterized systematically with high-fidelity.

For the sake of thermal conductivity improvement on CNT aerogel and mat, with comprehensive understanding on constitution of CNT aerogel, growth parameters during FCCVD have been optimized to get longer individual CNTs before forming a CNT aerogel, which was believed to offer a better heat conduction pathway in CNT aerogel. Moreover, with state-of-the-art steady state thermal conductivity measurement system, we will also show the thermal conductivity modification influence of decorated hexagonal boron nitride nanoflakes on CNTs.

These results will aid in fully realization of perfect individual CNT properties in the CNT aerogel, especially optimization of CNT aerogel thermal properties, so that applications of CNT aerogel can be explored and implemented in sectors such as the automotive and aeronautic industries.

4OF.1

A Review of Radical Chemistry in Oxidation Flow Reactors for Atmospheric Chemistry Research. ZHE PENG, Jose-Luis Jimenez, *University of Colorado-Boulder*

Oxidation flow reactors (OFR) use oxidants at higher-than-ambient concentrations to simulate atmospheric oxidation processes in shorter experimental times than in the atmosphere. The most common OFR type is, by far, uses OH produced by photolysis of H_2O and/or O_3 at using Hg lamp emissions at 185 and/or 254 nm. Because of its portability and promise as an alternative to environmental chambers, as well a recent commercial availability, the use of this type of OFRs in both lab and field is increasing extremely rapidly, and may result in a publication output comparable to that of large chambers in a few years. However, since its oxidant generation is similar to stratosphere, skepticism about the relevance of the chemistry OFRs simulate tropospheric oxidation has persisted in the atmospheric chemistry community. During last few years, a series of studies have been carried out to comprehensively investigate the radical chemistry in OFRs, under what conditions it is tropospherically relevant. We will present a review of recent studies on this topic, with a focus on providing OFR experimentalists with clear guidance about inputs and operating procedures to employ and avoid. First, the radical chemistry of HO_x, NO_y, and organic peroxy radicals (RO_2) in OFRs is discussed in terms of their production and loss. OFR conditions are often similar to those in the troposphere as OH dominates against undesired non-OH effects. The key reason why some conditions lead to tropospherically irrelevant/undesired processing of volatile organic compounds (VOCs) is that under some conditions, OH is drastically reduced while non-tropospheric/undesired VOC reactants are not. Common non-tropospheric/undesired VOC reactants are 185 and 254 nm photons, O atoms ($O(^1D)$ and $O(^3P)$), NO_3 etc. For each of these reactants, we summarize the conditions that enhance their relative importance to OH and the proposed approaches to avoid them, which allow improved OFR experimental design. We also review measures to realize specific experimental goals, the most important one of which is to achieve high-NO conditions. In addition, a number of related experimental issues are discussed, e.g., non-uniformity of UV field, possibility of particle charging by UV, and OH quantification at high precursor and/or aerosol mass loading. In this review, the latest version of estimation equations and OFR Exposure Estimators have been developed and made freely available, and will be briefly described.

4OF.2

Chemical Composition of Secondary Organic Aerosol Generated from Emissions of California Sage Plants Using a FIGAERO-ToF-CIMS. ARCHIT MEHRA, Jordan Krechmer, Andrew Lambe, Chinmoy Sarkar, Leah Williams, Fatemeh Khalaj, James Allan, John Jayne, Hugh Coe, Douglas Worsnop, Celia Faiola, Manjula Canagaratna, *University of Manchester*

Emissions from plants are the main source of atmospheric biogenic volatile organic compounds (BVOCs). Oxidation of BVOCs under ambient conditions results in formation of more oxidised species, many of which have lower volatility than their precursors. These species can partition into the particle phase and contribute to secondary organic aerosol (SOA) formation. To date, the majority of laboratory biogenic SOA experiments have been focused on single or simple multi-component BVOC mixtures that are thought to be representative of Northern Hemispheric deciduous or mixed forest conditions; thus, gaps remain in our understanding of SOA formation from complex mixtures of real plant emissions in other environments. Towards the goal of understanding SOA formation of plant emissions in other source regions, we conducted a series of experiments where Black Sage (*Salvia mellifera*) and California Sagebrush (*Artemisia californica*) plant emissions (the most common plant species in southern California's coastal sage ecosystem) were oxidised in an Aerodyne Potential Aerosol Mass Oxidation Flow Reactor. The chemical composition and the volatility of the SOA were probed with a high-resolution time-of-flight chemical-ionization mass spectrometer equipped with a Filter Inlet for Gases and AEROsols (FIGAERO-ToF-CIMS). Chemical ionization was performed with the iodide reagent ion, which is sensitive to multifunctional oxidized species. Single-BVOC oxidation experiments were also performed with eucalyptol, camphor and camphene, which are the major constituents of the Sage plant emissions. Positive Matrix Factorisation of the FIGAERO-ToF-CIMS mass spectra was used to identify contributions of the individual VOCs to the emission profile of SOA generated from oxidation of the plant emissions. FIGAERO thermograms of SOA generated from standards and the real plant mixture will be presented with the PMF factor results and data interpretation.

4OF.3

Secondary Organic Aerosol Formation and Aging in a Flow Reactor in the Forested Southeast US during SOAS. WEIWEI HU, Brett Palm, Pedro Campuzano-Jost, Douglas Day, Suzane de Sá, Benjamin Ayres, Danielle C. Draper, Juliane L. Fry, Amber Ortega, Lina Hacker, Astrid Kiendler-Scharr, Aki Pajunoja, Annele Virtanen, Jordan Krechmer, Manjula Canagaratna, Samantha Thompson, Laxmi Narasimha Yatavelli, Harald Stark, Douglas Worsnop, Scot T. Martin, William Brune, Steven S. Brown, Jose-Luis Jimenez, *CIRES, University of Colorado, Boulder*

A major field campaign (Southern Oxidant and Aerosol Study, SOAS) was conducted in summer 2013 in a forested area in Centreville Supersite, AL (SEARCH network) in the southeast U.S. To investigate secondary organic aerosol (SOA) formation from biogenic volatile organic compounds (BVOCs), 3 oxidation flow reactors (OFR) were used to expose ambient air to oxidants and their output was analyzed by state-of-the-art gas and aerosol instruments including a High-Resolution Aerosol Mass Spectrometer (HR-AMS), a HR Proton-Transfer Reaction Time-of-Flight Mass Spectrometer (PTR-TOFMS), and two HR-TOF Chemical Ionization Mass Spectrometers (HRToF-CIMS). Ambient air was exposed 24/7 to variable concentrations of each of the 3 main atmospheric oxidants (OH, NO_3 radicals and O_3) to investigate the oxidation of BVOCs (including ambient isoprene-derived epoxydiols, IEPOX) and SOA formation and aging. Effective OH exposures up to 1×10^{13} molec cm^{-3} s were achieved, equivalent to over a month of aging in the atmosphere, although the peak SOA formation was observed for equiv. exposures of about 1 day. Multiple oxidation products from isoprene and monoterpenes including small gas-phase acids were observed in OH OFR. High SOA formation of up to 12 $\mu g\ m^{-3}$ above ambient concentrations of 5 $\mu g\ m^{-3}$ was observed under lower OH exposures, while very high OH exposures led to destruction of ~30% of ambient OA, indicating shifting contributions of functionalization vs. fragmentation, consistent with results from urban and terpene-dominated environments. The highest SOA enhancements were 3-4 times higher than ambient OA. More SOA is typically formed during nighttime when terpenes are higher and photochemistry is absent, and less during daytime when isoprene is higher, although the IEPOX pathway is suppressed in the OFR. SOA is also observed after exposure of ambient air to O_3 or NO_3, although the amounts and oxidation levels were lower than for OH. Formation of organic nitrates in the NO3 oxidation will also be discussed.

4OF.4

Missing Ozone-Induced Potential Aerosol Formation in a Suburban Deciduous Forest near Tokyo. TOMOKI NAKAYAMA, Yuuki Kuruma, Yutaka Matsumi, Yu Morino, Kei Sato, Hiroshi Tsurumaru, Sathiyamurthi Ramasamy, Yosuke Sakamoto, Shungo Kato, Yuzo Miyazaki, Tomoki Mochizuki, Kimitaka Kawamura, Yasuhiro Sadanaga, Yoshihiro Nakashima, Kazuhide Matsuda, Yoshizumi Kajii, *ISEE, Nagoya University*

As a new approach to investigating formation processes of secondary organic aerosol (SOA) in the atmosphere, ozone-induced potential aerosol formation was measured in summer at a suburban forest site surrounded by deciduous trees, near Tokyo, Japan. After passage through a reactor containing high concentrations of ozone, increases in total particle volume (average of 1.4×10^9 nm^3/cm^3, which corresponds to 17% that of pre-existing particles) were observed, especially during daytime. The observed aerosol formations were compared with the results of box model simulations using simultaneously measured concentrations of gaseous and particulate species. According to the model, the relative contributions of isoprene, monoterpene, and aromatic hydrocarbon oxidation to SOA formation in the reactor were 24, 21, and 55%, respectively. However, the model could explain, on average, only about 40% of the observed particle formation, and large discrepancies between the observations and model were found, especially around noon and in the afternoon when the concentrations of isoprene and oxygenated volatile organic compounds were high. The results suggest a significant contribution of missing (unaccounted-for) SOA formation processes from identified and/or unidentified volatile organic compounds, especially those emitted during daytime. Further efforts should be made to explore and parameterize this missing SOA formation to assist in the improvement of atmospheric chemistry and climate models.

4OF.5

Using a Mobile Laboratory Equipped with an Oxidative Flow Reactor to Study Oxidative Aging of In-use Motor Vehicle Emissions. KEREN LIAO, Qi Chen, Yan Zheng, Ying Liu, Tong Zhu, *Peking University*

Vehicle emissions in megacities like Beijing contribute a large amount of gaseous precursors that can form secondary organic aerosol (SOA) via atmospheric oxidation. The contribution of SOA formation from vehicle exhaust to ambient particulate matter concentrations however remains unclear. Most of the current chemical transport models are unable to reproduce the magnitude and the variability of SOA mass in urban regions, suggesting large uncertainties in the emission inventories and/or in the SOA formation mechanism. For the transportation sector, it is important to investigate the SOA formation under actual driving conditions of traffic fleets which has not been studied before in China. We therefore deployed a Potential Aerosol Mass (PAM) flow reactor in a mobile laboratory to investigate the in situ SOA formation from in-use motor vehicle emissions on the major roads in Beijing in 2018. Vehicle exhaust is sampled and delivered into the PAM reactor periodically. The hydroxyl radical exposure in the PAM reactor is cycled from ~ 1 to 10 days of equivalent atmospheric oxidation. Concentrations of traffic-related gaseous precursors and some oxidation products are measured by gas analyzers and a proton transfer reaction mass spectrometer. Chemical composition of fine particles is measured by a time-of-flight aerosol chemical speciation monitor equipped with 2.5-µm lens and a capture vaporizer. The observations are discussed on the basis of the source apportionments of ambient particles from a long-term site. Potential contribution of mobile sources to fine-particle concentrations is estimated.

4OF.6

Evolution of the Complex Refractive Index of Secondary Organic Aerosols during Atmospheric Aging. QUANFU HE, Nir Bluvshtein, Lior Segev, Daphne Meidan, Michel Flores, Steven S. Brown, William Brune, Yinon Rudich, *Weizmann Institute of Science*

Secondary organic aerosols (SOA) from biogenic and anthropogenic sources represent a large fraction of the tropospheric aerosol mass. The optical properties of SOA can vary as a function of wavelength, but only a few studies have reported measurements of the wavelength-dependent aerosol extinction cross section and complex refractive indices, particularly in the visible spectral range. Additionally, there is a large knowledge gap of how the optical properties of SOA in the visible spectral region evolve as a function of atmospheric aging. To address this issue, we applied a novel laboratory instrument to measure aerosol extinction as a function of wavelength from 400 to 650 nm, using a white light-broadband cavity enhanced spectroscopy (BBCES). The instrument was validated by measuring CO_2 Rayleigh scattering cross section and extinction of reference materials. The new system was used to measure the changes in the optical properties of β−pinene and *p*−xylene SOA produced and aged in an oxidation flow reactor (OFR), simulating daytime aging by OH radical exposure under NOx-free conditions. It was found that these SOA are not absorbing in the visible range, and the real part of the refractive index (RI), n, for these two types of SOA showed slight spectral dependence in the visible range. With increased OH exposure, n first increased and then decreased, possibly due to an increase in aerosol density and chemical mean polarizability for SOA produced at low OH exposures, and a decrease in chemical mean polarizability for SOA produced at high OH exposures, respectively. A simple radiative forcing calculation suggests that atmospheric aging can introduce more than 40% uncertainty due to the changes in the RI for aged SOA.

4OF.7

Investigation for the Formation of Secondary Aerosol from Passenger Vehicles by Fuel Types (Gasoline, Liquefied Petroleum Gas, and Diesel). GYUTAE PARK, Sung-Woon Jung, Jounghwa Kim, Seok-Jun Seo, Sunmoon Kim, Kyunghoon Kim, Taekho Chung, Taehyun Park, Heekyoung Hong, Sunhee Moon, Seokwon Kang, Seung Hwan Lee, Min Seok Song, Jihee Ban, Dong-Gil Yu, Youdeog Hong, Taehyoung Lee, *Hankuk University of Foreign Studies*

Recent research proposed that Secondary Aerosol (SA) formation in the atmosphere impacts on air pollution and health effects. However, there has been lack of studies to investigate SA formation all over the world. This study tried to focus on understanding potential mass formation between primary and secondary aerosol by chassis dynamometer for in-use vehicle. The study on potential aerosol formation from different vehicle's fuels was conducted at the facility of Transport Pollution Research Center (TPRC), National Institute of Environmental Research (NIER), Korea. Three different types of fuels such as gasoline, liquefied petroleum gas (LPG) and diesel were tested on the FTP-75 and NEDC driving mode. An oxidation flow reactor (OFR) used in the study was the Aerodyne Potential Aerosol Mass (PAM) flow reactor. The PAM reactor is a cylindrical camber 46 cm long and 22 cm ID with a volume of approximately 13.3 liters. Two UV lamps (185 and 254 nm) are used to produce oxidants (O3, OH, and HO2) in the PAM (referred to as the OFR-185 method), or OH production from photolysis of injected (externally produced) O3 using 254 nm UV lamp (referred to as the OFR-254 method). In this study, OFR-254 method was operated with a residence time in the range of 1-2 min. During the study, relative humidity (RH) and temperature were under 25% and 30℃. Chemical composition of aerosol from vehicle emission and through PAM was measured by the High Resolution-Time of Flight-Aerosol Mass Spectrometer (HR-ToF-AMS). The HR-ToF-AMS provides non-refractory aerosol mass concentrations including nitrate, sulfate, hydrocarbon-like and oxygenated organic aerosol in real time.

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4OF.8

Comparison of Composition and Volatility of Soa Formed from Oxidation of α-Pinene and Scots Pine Emissions. ARTTU YLISIRNIÖ, Angela Buchholz, Claudia Mohr, Andrew Lambe, Celia Faiola, Eetu Kari, Taina Yli-Juuti, Sergey Nizkorodov, Douglas Worsnop, Siegfried Schobesberger, Annele Virtanen, *University of Eastern Finland*

Secondary organic aerosol (SOA) formed via oxidation of volatile organic compounds (VOCs) is composed of numerous chemical compounds with different functionalities. These compounds dictate chemical and physical properties of the particles, such as hygroscopicity, viscosity and density. A major part of the chemical complexity of SOA stems from the diversity of the initial VOCs and how these compounds are exposed to different oxidative conditions.

In this study, we investigated how differences in oxidative conditions alter volatility and composition of resulting SOA, when particles were formed from oxidation of either α-pinene or Scots Pine VOC emissions. VOCs were introduced into an Aerodyne PAM oxidation flow reactor (OFR). Volatility and composition of the formed SOA particles were measured utilizing a filter inlet for gases and aerosols on a time-of-flight chemical ionization mass spectrometer (FIGAERO-ToF-CIMS) using iodide ionization. The particles were additionally monitored with an Aerodyne aerosol mass spectrometer (AMS). VOC emissions from Scots Pine seedlings were monitored by proton transfer reaction and gas chromatography mass spectrometry (PTR-ToF-MS, GC-MS).

For α-pinene emissions, we used three different oxidative conditions in increasing trend of oxidative strength termed “low”, “medium” and “high”. Due to varying emission profile from Scots Pines we used fixed oxidative conditions comparable to “medium” case in three separate tree emission experiments and stronger oxidative conditions in one tree emission experiment. The α-pinene results show clear correlation between strength of oxidative conditions and volatility of the resulting SOA: The volatility of the particle phase decreased by ~3 orders of magnitude and approximate O:C increased from 0.65 to 0.9 as the level of oxidative exposure increased. The Scots Pine experiments demonstrate the importance of sesquiterpenes in the oxidation processes as emissions from the trees consisted of 20-50 % sesquiterpenes by mass concentration, which are within the range of values measured from Scots pine emissions in the field. The sesquiterpene-influenced SOA had lower volatility than for any of the α-pinene experiments, even when resulting from oxidative conditions comparable to “medium” exposure.

These results are important for understanding formation and transformation of SOA particles in the atmosphere, since coniferous tree emissions are often assumed to be mostly α-pinene and other monoterpenes.

4OF.9

Volatility Distribution of Primary Organic Aerosol from Food-Cooking Emissions and Its Evolution upon Oxidation.

MANPREET TAKHAR, Arthur W. H. Chan, *University of Toronto*

Food cooking emissions represent one of the most important sources of primary organic aerosol (POA) in urban areas and have been shown to contribute 10-34% of total organic aerosol. However, the evolution of cooking emissions in the atmosphere is not fully understood. The gas-particle partitioning of cooking-related organic compounds is largely determined by their vapor pressures and volatilities, which can also have a significant impact on aerosol chemistry. In this work we study the volatility distribution of primary and secondary organic aerosol (P/SOA) from cooking emissions. We use cooking oils (canola oil, olive oil, peanut oil) as a surrogate to investigate the chemical composition and volatility using thermal desorption-gas chromatography mass spectrometry (TD-GC/MS), and a thermodenuder. In particular, we focus on the composition of intermediate volatile organic compounds (IVOCs) emitted from food-cooking emissions. Heated cooking oil particles were oxidised in a quartz flow tube reactor in presence of ozone or hydroxyl radicals to simulate atmospheric aging. Tenax tube samples and quartz filter samples were collected for analysis of IVOCs and particle-phase organics. We hypothesize that the overall volatility of oxidised cooking aerosol decreases upon oxidation due to addition of functional groups.

The unoxidized cooking emissions were found to be mainly comprised of saturated fatty acids ranging from C12-C20, along with palmitoleic acid, oleic acid, linoleic acid and sterols. The oxidised cooking emissions were comprised of dicarboxylic acids, hydroxy fatty acids, and short chain fatty acids. The organic compounds are therefore becoming more functionalized upon oxidation as hypothesized. The vapour pressures of organic compounds identified in cooking oil samples were estimated based on GC retention times and compared to the temperature dependent volatility distribution measured using the thermodenuder. Upon oxidation, the thermodenuder showed a decrease in the overall volatility as indicated by increased mass fraction remaining at high temperatures. However, the organic compounds identified using GC/MS are smaller and have higher vapor pressures. The inconsistency between the thermodenuder and GC/MS results could be ascribed to a few reasons. The first is the fragmentation of higher molecular weight compounds in the TD-GC/MS due to high desorption temperatures, thus leading to higher apparent volatility. Another possible explanation is the change in the morphology of the particles upon oxidation. Upon oxidation the particles may become sufficiently viscous to hinder evaporation or growth. Thus, while the compounds become more volatile, they also become more difficult to evaporate upon heating. The mass transfer limitations within the particle were investigated using thermodenuder mass transfer models to evaluate the significance. Overall, our results highlight the need to understand both the chemical composition and the particle-phase state to understand the evolution of cooking emissions in the atmosphere.

4OF.10

Assessment of a Field Portable Oxidation Flow Reactor (OFR) Measurement System for Biofuel Emission Characterization in Remote and Rural Settings. ADITYA SINHA, Andrew Grieshop, *North Carolina State University*

Oxidation flow reactor (OFR) experiments in our lab have explored the properties of secondary organic aerosol (SOA) formed from photochemical aging of emissions from cookstoves like those used by billions daily. Lab experiments have explored the physical and chemical properties of SOA formed from emissions for stove types of varying efficiencies, different fuel types (hard and soft wood) and various operating OFR conditions. The OFR simulated up to 18 days of equivalent atmospheric aging and we observed peak organic aerosol (OA) enhancements of about a factor of 3 over primary OA, dependent on stove and fuel types. However, field emission monitoring efforts have consistently shown a clear distinction between in-field performance of cookstoves and that from standardized lab tests. For instance, the primary particulate matter emission factors (PM EFs) measured in the field are often 2 or more times that in the lab[1]. The work presented here builds on previous experiments to develop simplified methods to quantify SOA formation potential from emissions during in-home use of biomass stoves. Typical lab experiments have characterized cookstove emissions utilizing sophisticated instrumentation like the Aerosol Chemical Speciation Monitor (ACSM) and Photoacoustic Extinctiometer (PAX). Since the ability to move and power advanced instruments is limited in remote and rural locations, we are developing an ensemble consisting of portable low power instruments to measure components of interest. We will evaluate this field-portable sensor suite – consisting of optical PM sensors measuring scattering/absorption, CO and CO2 sensors, and filters alongside corresponding lab based instrumentation to assess performance for international rural applications.

Preliminary evaluation indicates that OA enhancement, quantified in the lab using an ACSM correlates fairly well with the enhancement in light scattering coefficient (Bscat), quantified using a PAX. We observe a linear relationship between the OA enhancement and Bscat Enhancement across a range of stove efficiencies, fuel types and aging conditions. This indicates a potential to measure OA enhancement in real time with a portable sensor capable of measuring light scattering. We expect a high degree of inter-test variability in field measurements (for example, organic carbon emissions factors, OC EFs vary by a factor of 2-4[1]) and so it is useful to have a measurement metric that can capture a range of enhancements (up to a factor of 2.8 based on lab testing) across aging equivalent to atmospheric exposure of 1 to 18 days. Filters are a standard method for determining PM, OC and elemental carbon (EC) EFs from a combustion event. In prior lab cookstove emission OFR experiments, we evaluated closure between PM from filters and parallel ACSM measurements. In these comparisons, filters under-predict the OA EFs relative to the ACSM, and so further work is required to evaluate the use of filters for measuring aged OA from an OFR. A hypothesis to be tested is that residual ozone from the OFR, (not fully denuded prior to reaching filters) interacts with and degrades filter-bound organic matter. Experiments will be designed to probe this disparity since filters are often a relatively inexpensive and operationally efficient way to gather important descriptors of OA from a combustion event. Subsequent steps will involve deployment of the OFR along with the measurement suite during the summer of 2018 in Mexico in a rural and remote setting.

References:
[1] Grieshop, A. P., G. Jain, K. Sethuraman, and J. D. Marshall (2017), Emission factors of health- and climate-relevant pollutants measured in home during a carbon-finance-approved cookstove intervention in rural India, GeoHealth, 1, 222–236, doi:10.1002/2017GH000066.

4OF.11

Well Mixed, Ambient Conditions and Long Observation Times: Aging Experiments in a CSTR. FRANZ FRIEBEL, Amewu Mensah, *ETH Zürich*

Aerosol particles which are emitted into the atmosphere are exposed to different reactants and therefore change their properties. The average atmospheric lifetime ranges from several hours to more than a week. Experimental approaches which investigate the occurring changes in aerosol particle properties should ideally cover these time scales. Generally, there are two approaches to mimic these time frames. One, the concentration of reactants, e.g. Ozone or OH-radicals can be increased to trigger faster reaction rates e.g. Potential Aerosol Mass (PAM) Oxidation Flow Chambers. Two, larger aerosol tanks can be constructed to extend the observation time e.g. AIDA-Chamber at KIT. Both approaches imply their specific challenges. Treating aerosols with high concentrations of oxidants bears the risk that atmospheric processes are not represented well. An example is the heterogenous oxidation of soot particles with ozone, where the reaction mechanism follows a Langmuir-Hinshelwood kinetic where an elevated ozone concentration does not lead to a faster reaction. Extending the observation time by extending the tank volume is often technically and financially challenging.

Here we present an approach that makes use of the continuously stirred tank reactor (CSTR), a concept well known in chemical engineering but rarely applied in atmospheric science. This approach decouples long observation times from high chamber volumes thereby allowing low reactant concentrations and low aerosol flows.

Generally, aerosol tanks get filled once and provide a flow of aged aerosol until the reservoir is exploited (batch mode). In contrary to that, the CSTR aerosol tank is continuously filled with fresh aerosol and provides a constant sample flow over an unlimited time scale after the tank reached steady state conditions. The sample flow does not consist of a uniform aerosol sample but of a mix of aerosol samples at different aging stages. Nevertheless, statistical challenges in subsequent data analysis can be disentangled by incorporation of the well-defined aerosol age distribution.

From Summer 2016 till winter 2017/18 we conducted several lab campaigns at ETH Zurich where we successfully applied the CSTR aerosol tank concept. Size selected soot particles were exposed to different ozone concentrations (0-200 ppb), at a temperature range of 5°C to 35°C and at different levels of humidity (0-80%) in a 3 m3 stainless steel tank. The setup generated a sample flow of 25 lpm and allowed several instruments to measure the identical and undiluted sample flow for up to 16 h.

An increase of ozone gas phase concentration by a factor of 10 results in a reduction of CCN activation time of only 1.7. At the contrary, a reaction temperature increase of 10 K results in a decrease of activation time by a factor of 1.5 - 2.0. Here, we focus on the underlying principles of CSTR-data analysis and present the advantages of this experimental approach allowing for new insights into atmospheric ageing processes.

4RA.1

Atmospheric Nanoparticle Dry Deposition Velocity. PHILIPPE LAGUIONIE, Luc Solier, Denis Maro, Geoffrey Pellerin, Didier Hébert, Olivier Connan, Oumar-Telly Bah, *IRSN*

In the context of accidental release of radioactive particles into the atmosphere, knowing atmospheric particle dry deposition velocities on ground surfaces is essential to assess risks both on populations and environment. The dry deposition velocity (m s^{-1}): (1) is the ratio of deposition flux (# m^{-2} s^{-1}) over atmospheric concentration (# m^{-3}); (2) has a general applicability as it does not depend on #-entity; (3) depends on the deposition process integrating time-step. The dry deposition velocity depends on the aerosol particle diameter. Currently, there is no in situ dry deposition velocity available in the literature for nanoparticles, whereas it is required to predict deposition of radionuclides as, for examples, ruthenium-106 and iodine-129,131 (reactive gas). In this framework, one of the main challenges is to find a suitable tracer to follow atmospheric nanoparticle deposition at short time scales. In this study, we tested the capability of the naturally-occurring radionuclide bismuth-214 (^{214}Bi, beta emitter, $T_{1/2}$ = 19.7 min) to trace the deposition flux of the atmospheric nanoparticles at hour scale over a grassland (ABBA project, June 2017). ^{214}Bi is a decay product of radon-222 (^{222}Rn, $T_{1/2}$ = 3.8 days) emitted by terrestrial natural radionuclides. ^{214}Bi activity was assumed to be the same as its daughter polonium-214 (alpha emitter, $T_{1/2}$ = 1.6 10^{-4} s) that was quickly counted by a multichamber alpha spectrometer (Canberra, model 7401) located in a mobile lab. Vertical fluxes were calculated using the activity concentration gradient method from samplings on diffusive grids located at 0.7 and 2.7 m above grass. Next, atmospheric activity concentrations were calculated from grid activities using the Jenkings equations. Results showed a significant dry deposition velocity normalized by the shear velocity of 0.06 ± 0.03.

4RA.2

Observational Evidence of Downdraft Clouds Contributing to Daytime Elevated Nitrate Concentration in an Urban Atmosphere. Jun Tao, Zhisheng Zhang, LEIMING ZHANG, Yunfei Wu, Junji Cao, Peng Cheng, Laiguo Chen, Renjian Zhang, *South China Institute of Environmental Sciences*

Nitrate has become the most important hydrophilic chemical component in $PM_{2.5}$ during serious air pollution periods in urban areas of Pearl River Delta (PRD) region of south China, but there is a lack of fully understanding of its formation mechanisms and controlling factors, especially during daytime nitrate episodes. To fill the knowledge gap, water-soluble inorganic ions in $PM_{2.5}$ and trace gases including SO_2, HNO_3, NH_3, NO_x and O_3, particle size distribution, vertical distribution of aerosol backscatter density, and selected meteorological factors were synchronously measured at high time resolution at an urban site in PRD. The remarkably enhanced nitrate mass concentration during daytime were identified to be caused by downdraft cloud processes and related cloud recycling and evaporating of atmospheric aerosols. Cloud downdrafts enhanced more of nitrate and ammonium than sulfate concentrations in ambient air, a finding that may have important implications on the sources of secondary inorganic aerosols in this and other similar cloudy regions.

4RA.3

Aerosols Characterization in Upper Egypt; Urban and Rural Measurements. MOSTAFA MOSTAFA, Hyam Khalaf, Mona Moustafa, Amer Mohamed, *Ural Federal University*

Abstract Mass size distribution of aerosol particles and the elemental composition of Particulate Matter (PM) were examined in rural and urban areas in El-Minia governorate, Upper Egypt. Low pressure Berner cascade impactor was used to collect aerosol particles. Seven elements were investigated including Ca, Ba, Fe, K, Cu, Mn and Pb using atomic absorption technique. Measurements were performed in El-sharyna village representing a rural site and Maghagha city representing an urban site in El-Minia governorate. Meteorological parameters (temperature and relative humidity) were recorded during the sampling. Elemental mass size distributions were founded as a bi-modal log normal distribution corresponding to accumulation and coarse modes. The mass concentrations of the measured elements ranged from 0.58 ng/m3 (for Ba) to 108.7 ng/m3 (for Fe) at El-sharyna village. The mass concentration at Maghagha city ranged from 0.05 ng/m3 (for Ba) to 96.8 ng/m3 (for Fe).

4RA.4

Vertical and Horizontal Distribution of Sub-micron Aerosol Chemical Composition and Physical Properties across Northern India, during the Pre-monsoon and Monsoon Seasons. JAMES BROOKS, Hugh Coe, William Morgan, James Allan, Paul Williams, Dantong Liu, Jim Haywood, Cathryn Fox, Justin Langridge, Ellie Highwood, Suresh Babu, S.K. Satheesh, Andrew Turner, *University of Manchester*

The Indian subcontinent is one of the most polluted regions in the world. At the moment, the nature and magnitude of the aerosol impacts are poorly understood and constrained. Uncertainties lie in the vertical distribution, spatial distribution of various different aerosols and the relative contribution from different sources (Chakraborty et al, 2016).

The South West Asian Aerosol-Monsoon Interactions (SWAAMI) project, which occurred from June to July 2016, sought to address these uncertainties by carrying out an airborne experiment. Such experiment was on-board the UK Facility for Airborne Atmospheric Measurements (FAAM) BAe-146 research aircraft. The field campaign conducted 22 flights in advance of the summer monsoon, and during the onset phase. The vertical and spatial extent of aerosols were studied across both Northern India (based out of Lucknow, in the Indo-Gangetic Plain (IGP)) and in Southern India (based out of Bangalore). Two aerosol instruments were operated by the University of Manchester on-board the aircraft; an Aerodyne Aerosol Mass Spectrometer (AMS) and a DMT Single Particle Soot Photometer (SP2).

In the IGP, organic aerosol (OA) dominates the aerosol burden, whereas outside the IGP, sulphate dominates. BC mass concentrations indicate greater values inside the IGP. The main inorganic components show different spatial patterns; sulphate is regional in nature, especially in the pre-monsoon season. Nitrate appears to be determined by thermodynamic processes, with increased nitrate mass concentration in conditions of lower temperature and higher relative humidity. The total aerosol mass concentrations display decreases as monsoon rainfall arrives over the study regions. However, the decrease is less significant over the IGP, possibly indicative of the strength of emissions sources over this region. Inside the IGP the aerosol species are more absorbing in nature, whereas in NW India aerosol present is larger in size.

The aerosol mass concentration also displays variations in the vertical profiles. Inside the IGP, profiles undergo changes with monsoon progression. During the pre-monsoon, OA and absorbing aerosol species dominate in the lower atmosphere (<1.5km) with sulphate and scattering aerosol species dominating in an elevated aerosol layer (EAL) above (>1.5km). As the monsoon progresses into the IGP region, this EAL structure diminishes, with the profile decreasing in vertical extent, mass concentration and a switch to being dominated by OA. Outside the IGP, the profiles display sulphate aerosol dominating throughout, with no change in chemical composition with monsoon progression (only decrease in vertical extent and mass concentration throughout). Dust is present in the atmospheric column, with large concentrations in NW India and the IGP. The dust concentrations decrease significantly in the IGP due to removal by the monsoon rainfall. These results will serve as useful model input for the SE Asia region.

This work was supported by the National Environmental Research Council (NERC) under grant NE/L002469/1.

Reference: Chakraborty, A., Gupta, T. and Tripathi, S. N. (2016) Atmospheric Environment 136 144-155.

4RA.5

Predicting Wildfire in United States Using Artificial Neural Network Technique. KAIYU CHEN, Hao Guo, Hongliang Zhang, *Louisiana State University*

Wildfire is the largest source of air pollutants such as particulate matters and toxins, which greatly changes landscape with impacts on human health, large scale climate changes, social economy and ecosystem in the U.S. In this study, Artificial Neural Network (ANN) is applied to simulate the risk of wildfire in the U.S. based on the date recorded from 2000 to 2016. Relationship between wildfire activities, represented by fire occurrence and its brightness and fire radiative power (FRP), with climate factors including temperature (TEM), relative humidity (RH), wind speed (WS) and wind direction (WD) was simulated. Trained by using observation date, our model is reliable to show correlation between climate factors and wildfire activities. Via this model, we are able to estimate fire by detecting climate conditions from closest meteorology station. Results from this study could provide information for wildfire prediction, prevention and controlling management.

4RA.6

Investigation of the Morphology and Chemical Composition of Intra-Urban Atmospheric Particles: Case Study of Tehran, Iran. Balal Oroji, Asghar Sadighzadeh, Eisa Solgi, HOSSEIN YOUSEFI, *Nuclear Science and Technology Research Institute, Iran*

Nowadays, air pollution in cities with regard to its harmful outcomes has been turned into one of the serious challenges in urban management and Tehran city, one of the most polluted cities in the world. As the air pollutant gases concentration is being influenced by environmental factors, the probability of pollution will not be uniform across Tehran. The work described the use of Scanning Electron Microscopy (SEM) combined with X¬-ray Dispersive Energy Spectrometry (EDS) to characterize inorganic atmospheric particles samples collected on PM10 filters from June to October 2017 from five zones within the city of Tehran. Given the wind direction in the region, the particles produced in the urban areas move to the east and north-east during most of the autumn. These particles grow at the time of displacement when dealing with a single-rod and are eliminated with increasing weight when dealing with different levels. Due to the nature of these particles and their subterranean nature, the risk of inhaling particles in the center of the area to the east of the region is more than other areas. The elemental composition of these particles indicates that C, O and Si rich particles were dominant. The other dominated elements were Zn, Ca and Al. This could be inferred as the fly ash origin. These particles can be related to originate from construction activity, regional transport from the urban zones as well as agricultural vegetative burning and natural dust. These particles are composed primarily of feldspar (Ca, Si, Al) and clay (Al, Fe, Si), their origin is mainly crustal, but they can also come from erosion of building products and road dust. Our results indicate that in autumn and winter, the air quality at Tehran is often influenced by regional air pollution as shown by spatial distribution of PM10 concentration. It is found that PM10 had almost the same concentration in regional background air and in different types of urban environments. The special meteorological conditions and the role of regional-scale transport can explain why local abatements in cities cannot lead to significant improvement of the air quality during smog events. These particles morphology and chemical composition, illustrate an abundance of natural elements within the zone. However, some of the elements presented are directly related with human activities, and are of much interest from the public health and environmental perspectives. Due to atmospheric conditions in the region, the suspended particles in the atmosphere are divided into two major groups: urban particles that are the result of combustion of fossil fuels in the region. In the second group, resources are generated outside of the urban boundaries and in the marginal areas of the study area, which mainly consist of particles from dust storms, biomass, as well as moving and fixed resources. Land use change in the western regions of the region and the conversion of vegetation cover and rangelands to residential and industrial areas is the main reason for the production of pollutants in these areas. The shape of these particles is irregular due to the origin of the mineral and due to the presence of biomass particles; they are regular and sometimes spherical forms. Carbon and silica are mainly found in the composition of these particles.

4RA.7

Pollutant Measurements at Near Road and Background Sites. OLIVER RATTIGAN, H. Dirk Felton, Brian P. Frank, *New York State Dept. of Environmental Conservation*

Public concern about the heightened exposure to near-roadway (NR) pollutants had led to a national near-roadway air monitoring program. In New York State monitoring has been ongoing at three urban NR locations. Pollutants measured at these sites include PM2.5 mass, Nitrogen Oxides (NO, NO2, NOx), Ultrafine Particles, Black Carbon (BC) and CO. Measurements at NR sites are usually made in conjunction with existing urban background sites. In general, pollutant concentrations are elevated at the near road site compared to the background site particularly during the daytime hours. At Rochester for example BC at the near roadway site is elevated by a factor of 2.0-3.0 between 7AM and 3 PM dropping to near uniform concentrations at night. The enhancement in BC is highest in summer and lowest in winter. Other co-pollutants including NOx, CO and PM2.5 mass are also elevated at the NR site by varying degrees during daytime hours. The data are used to determine diurnal, weekday/weekend and seasonal patterns. Pollutant source direction is determined through nonparametric wind regression. The data will be used to determine compliance with National Ambient Air Quality Standards.

4RA.8

Source Apportionment and Associated Oxidative Potential of Ambient PM in Beirut during Saharan and Arabian Dust Events. CHRISTOPHER LOVETT, Mohammad Sowlat, Najat A. Saliba, Alan Shihadeh, Constantinos Sioutas, *University of Southern California*

In this study, we examine possible changes in the oxidative potential of airborne particulate matter (PM) in Beirut, Lebanon, as well as the source apportionment of this PM redox activity, that occur during dust events originating in the Sahara and Arabian deserts. Segregated fine (< 2.5 µm) and coarse (2.5-10 µm) PM samples collected during dust events, as well as during non-dust periods, were analyzed for chemical composition and an in vitro alveolar macrophage assay was performed to determine their oxidative potential. To examine changes in the source apportionment of PM oxidative potential during dust events, we first conducted a bivariate correlational analysis of the compositional and biological data to calculate Spearman's rho coefficients. The correlational data indicating associations between PM components and oxidative potential were then used to perform principal components analysis (PCA) of the PM components and then multiple linear regression (MLR) to apportion the measured oxidative potential to distinct source groups and compositional source factor scores. Our findings revealed that the oxidative potential of Beirut's urban PM during non-dust periods was much higher than during dust episodes, and the major contributors to this redox activity were traffic emissions combined with secondary organic aerosols (SOA). During days when aerosols from Saharan and Arabian dust events alter atmospheric PM composition, traffic emissions and SOA continued to dominate as sources of PM oxidative potential, along with the contribution of inorganic secondary ions (SI). The influence of dust aerosols on indigenous Beirut PM did not exacerbate its oxidative potential, thus suggesting that aerosols generated during Saharan and Arabian dust events pose no additional health risks to the population in that area.

4RA.9

Characteristics of Nuclei Mode Atmospheric Aerosol Particles during a Large Scale Fire Event. MANISH JOSHI, Mariam , Pallavi Khandare, Arshad Khan, B.K. Sapra, *Bhabha Atomic Research Centre, Mumbai*

Emission of trace gases and aerosol particles from large scale fires modify atmospheric aerosol characteristics. Such fires include biomass burning, forest fires, volcanic eruptions and accidental fires etc. (Chen et al. 2017; Jaffe and Wigder 2012). Large scale fires have potential to affect aerosol properties and consequently visibility, health and climate. This study focuses on measurements and interpreting modifications in number concentration and number size distribution in the size range 5-350 nm (measured by nano DMA/SMPS) during a large scale fire event (which took place during March 20-27, 2016 at a waste dumping ground in Mumbai, India). Sampling duration was segregated into case and control days and these characteristics were compared for interpreting effect of emissions due to fire on background aerosol characteristics, if any. Temporal evolution of integral number concentration showed several peaks, most of which coincide with simultaneous dip in geometric mean diameter. Data instances when the total number concentration was found to be more than 10^5 per cm^3 were≈ 1.8 % and 0.003% (of all data points) for case and control days, respectively. Similarly≈ 6.5 % and 5.3% times geometric mean decreased lesser than 20 nm for case and control days, respectively. On the days of fire event, formation of nuclei mode particles was noted during noon times. Size distributions for case days were easily differentiated from those of control days even if averaging was done for entire day. Further hourly averaged analysis revealed significant departure from background conditions during noon times only.

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4RA.10

Applications of Unmanned Aerial Systems in Atmospheric Environment Monitoring. ZHONG-REN PENG, Xiaobin Li, Dongsheng Wang, Bai Li, *Shanghai Jiao Tong University*

In recent years, unmanned aerial systems (UAS) and miniaturized sensors have been widely used to obtain atmospheric parameters within the lower troposphere. UAS platforms equipped with miniaturized sensors are capable of obtaining both vertical and horizontal distributions of air pollutants, which can be used in many aspects of the environmental science, such as air pollution forecasts and citizen exposure estimation. To explore potential utilization of the UAS platforms as much as possible, we have developed many types of UAS platforms (including fixed-wing and rotor-wing UAS) and used in many field experiments.

The measurement accuracy of UAS platforms under harsh operation environments of upper air was evaluated and calibrated with similar observation of a large tethered balloon platform that was equipped with standard air quality monitors. Results show that the UAS platforms were capable of accurately capturing both horizontal and vertical variations of air pollutants.

The fixed-wing UAS platforms were used to make observations of air pollutants (e.g. O_3 and $PM_{2.5}$) at three-dimensional scales within the 1000 m lower troposphere. Results show that observations of the fixed-wing UAS platforms can clearly demonstrate both vertical and horizontal variations of air pollutants, which can be used to analyze transport characteristics of air pollutants over the experimental area. The rotor-ring UAS platforms were also used to obtain vertical profiles of atmospheric parameters (e.g. O_3, $PM_{2.5}$, temperature, relative humidity, wind speed and wind direction) within the range of 0-1500 m. Observations of the rotor-ring UAS were capable of clearly demonstrating temporal variation patterns of atmospheric parameters, which helped analyze potential causes of air pollution events. Furthermore, the UAS platform was used to calibrate numerical models to obtain more accurate air pollution predictions.

4RA.11

High Temporal Resolution Analysis of Fine Particles Concentrations in 5D Virtual Space. LIBOR HEJKRLÍK, Helena Plachá, Dáša Richterová, *Czech Hydrometeorological Institute*

Number concentrations N of fine particles had been measured by SMPS in 7 channels (10–20 nm, 20–30 nm, 30–50 nm, 50–70 nm, 70–100 nm, 100–200 nm, 200–800 nm) with time resolution of one hour since June 2012 to December 2015 at a background urban site in Northern Bohemia. At the same measuring station of the National Air Pollution Network operated by the Czech Hydrometeorological Institute hourly means of three pollutants had been measured (mass concentrations of SO_2, NO_2 and PM_1 – black carbon). At two nearby climatological stations one-hour values of three meteorological elements were available (air temperature T_h, relative air humidity H_h and global radiation R_h). The whole period of observations covered 1309 days, periodically involving all of the seasons of the year with no respect to weekdays or rush hours. Night hours (R_h=0) were excluded even though they amounted to more than one half of available data. T_h varied between 11,2 °C and 36,1 °C, for H_h it was between 21% and 100% and R_h reached its extremes between 0,2 and 940,5 W/m^2. The maximum of mean concentration of SO_2 slightly exceeded the level 20 µg/m^3/hour, the highest value for NO_2 was registered at 100 µg/m^3/hour and PM_1 was mostly less than 14 µg/m^3/hour. Resulting number of analyzed rows of 5 variables (in two versions, one for SO_2 and another for NO_2) was approximately 14 000. The nearly-continuous combinations of meteorological data were transformed into THREE-DIMENSIONAL matrix where T_h, H_h and R_h were assigned only few discrete values (48, 13 and 13 respectively). In the resulting 8112 cells of the 3D matrix mean concentrations of the modes of fine particles were calculated. To clarify the whole picture only the cells containing at least 15 values of N were taken into account. The results were displayed in the form of XYZ bubble graph, diameters of the spheres being the FOURTH dimension. GrapherTM 11 (Golden Software, LLC) enables colouring of the bubbles regarding specific key, in this case one of four classes of mean hourly concentration of SO_2 or NO_2 in corresponding cells. The colour of the spheres may be regarded as the FIFTH dimension. The nucleation modes of nanoparticles (10–50 nm) demonstrate strong proliferation (N~10^4/cm^3/hour) under extreme both temperature and solar radiation while air moisture remains moderate. The overall picture changes for fine particles with diameter up to 800 nm. Their concentrations are one order less, the maximum values show considerable affinity to periods of low visibility and high humidity. They are possibly primary particles of anthropogenic origin; this is also supported by practically identical graphs for numeric concentrations of particles with diameter 200–800 nm and for mass concentrations of PM_1, obtained by MAAP instrument, it is by different physical method. Highest quantities of nanoparticles correlate with elevated concentrations of sulphur dioxide, whereas concentrations of NO_2 are low. The picture gradually fades out towards 50 nm limit probably due to advancing nucleation of sulphuric acid formed from the atmospheric oxidation of SO_2. Primary particles 50–800 nm reach their maximal values in correspondence with anthropogenically induced high concentrations of sulphur dioxide, probably of industrial origin as well as with elevated values of nitrogen dioxide that is a strong indicator of vehicle emissions.

4RA.12

Measurements and Analysis of Chemical Composition of Urban Aerosol during High Pollution Events at Guanzhong Plain, China.

Junji Cao, LIU HUIKUN, *Key Laboratory of Aerosol Chemistry and Physics, IEECAS*

Aerosol pollution is a serious environmental problem which influencing air quality, regional and global climates, and human health. Aerosol ($PM_{2.5}$) samples were collected at Guanzhong Plain, China with six sampling sites at different cities in the year scale from 2012 to 2014. All of the six sites exhibited highest organic carbon (OC) and elemental carbon (EC) values in winter and lowest values in summer. OC correlates well with EC indicating similar emission sources. The contributions of secondary species SO_4^{2-}, NO_3^- and NH_4^+ in total ions were greatest, and the high concentrations in winter were mainly due to emissions from coal combustion and biomass burning. During autumn the haze days were severest in Xi'an city with similar tendency of $PM_{2.5}$ variations, and it was proved that biomass burning may be the main emission source of the regional pollution. In winter pollution episodes, the pollution patterns in Guanzhong Plain were similar which was resulted from strong secondary reactions and coal burning.Source apportionment using a positive matrix factorization receptor model indicates that on average secondary aerosol was the main source of $PM_{2.5}$ (39.3%), followed by coal burning (17.3%), motor vehicle/industrial emissions (15.7%), fugitive dust (14.9%), and biomass burning (12.8%). The online, in situ measurement airborne species, especially the chemical composition of non-refectory submicron aerosol, during a heavy haze-fog event, was analyzed in detailed.The formation of secondary sulfate and organic aerosol were observed during the event. The sulfur oxidation ratio (SOR), defined as sulfate/(SO_2+sulfate) were mostly over 0.10, with a maximum of ~0.30, when relative humidity > 80%. The aging product of organic aerosol (OA) were also observed in the event. The wet scattering coefficient was influenced by secondary sulfate, in the form of $(NH_4)_2SO_4$, with contribution of 48.9% of wet particulate phase scattering. Thus decreased the visibility dramatically with a minimum of 128m. The current WRF-Chem model study suggested the secondary sulfate formation was essential to the increasing of sulfate concentration. The formation of secondary species was a decisive reason to form severe haze after fog event.

Keywords: $PM_{2.5}$, source appointment, chemical formation

4RA.13

Long Term Satellite Based Study on Aerosol and Trace Gases over the Capital City of Assam, Guwahati. JHUMA BISWAS, Papori Dahutia, *Pandu College, Guwahati, Assam, India*

The variability and trend in aerosol optical depth (AOD) by using the Moderate Resolution Imaging Spectroradiometer (MODIS) level 3 Collection 6 data at 550 nm for the period January, 2004 to December, 2016 and tropospheric columns of nitrogen dioxide (NO2) and sulfur dioxide (SO2) data by using Ozone Monitoring Instrument (OMI) has been studied for the period October, 2004 to December, 2016 over capital city of Assam, Guwahati. The monthly average AOD value varies from its highest value (0.63±0.09) in March to its lowest value (0.23±0.05) in October for the study period over Guwahati. The seasonally averaged AOD reached its maximum in pre-monsoon (0.61 ± 0.06), followed by winter (0.47 ± 0.07) and monsoon (0.41 ± 0.04), with the minimum occurring in post-monsoon (0.25 ± 0.06) season. The observed Ångström exponent value varies from its minimum value (1.18 ± 0.05) in monsoon season to its maximum value (1.35 ± 0.09) in post-monsoon season. Considerable long-term annual increasing trends in AOD, Ångström exponent and tropospheric NO2 column has been observed over the study location. An increasing trend of total number of vehicles along with their emissions degrades the air quality and thereby contributing to the increasing trend of AOD over Guwahati. A significant correlation between long term averaged MODIS AOD and OMI NO2 tropospheric columns with same seasonality indicating their same source of origination. Long term increasing trend in Ångström exponents (~0.008 per year) signify the contribution of smaller size aerosols attributed to urbanization and human activity over Guwahati. The monthly average visibility in Guwahati is highest (27.5 km) in October with a moderate reduction observed during the monsoon, reaching a minimum of 7.2 km in March. With increasing AOD values, horizontal visibility decreases over Guwahati.

4RA.14

Chemical Composition of PM2.5 in Zion, IL during the 2017 Lake Michigan Ozone Study. DAGEN HUGHES, Alissia Milani, Megan Christiansen, Dylan Millet, Timothy Bertram, Charles Stanier, Elizabeth Stone, *University of Iowa*

Areas along the coast of Lake Michigan are consistently in violation of federal air quality standards for ozone. The enhancement of ozone during the springtime and summertime is thought to result from the unique meteorology of coastal regions. In a collaborative effort to better understand ozone production over Lake Michigan, the Lake Michigan Ozone Study (LMOS 2017) took place from May 21 to June 23, 2017, combining airborne, ship, mobile lab, and fixed ground based measurements. Here, we focus on identifying the major sources contributing to fine particulate matter ($PM_{2.5}$) in Zion, Illinois so that the sources contributing to ozone formation can be better understood. Elemental and organic carbon (EC and OC), inorganic ions, organic molecular markers, and metals were quantified in daytime (08:00—20:00) and nighttime (20:30—07:30) ambient $PM_{2.5}$ samples. $PM_{2.5}$ mass concentration ranged from 1.2 – 11.5 $\mu g/m^3$ with an average concentration of 5.3 $\mu g/m^3$. OC levels ranged from <0.5 – 4.7 $\mu g/m^3$ (averaging 4.7 $\mu g/m^3$) while EC ranged from <0.05 – 0.8 μg/m3 (averaging 0.22 $\mu g/m^3$). The average OC:EC ratio was 12.25, suggesting a large contribution from secondary organic aerosol. The most significant contributor to $PM_{2.5}$ mass was organic matter (OM, calculated as 1.7 x OC, contributing 57.9%), followed by sulfate (16.4%), ammonium (6.3%), and nitrate (3.5%). Ozone concentrations exceeded the federal ozone standard of 70 ppb during a high-ozone event on June 02 and during a high-ozone period occurring from June 10 to June 16 where ozone concentrations reached 91 ppb and 88 ppb, respectively. The highest daily average of $PM_{2.5}$ mass occurred during the high-ozone event (10.7 $\mu g/m^3$) and was also elevated during the high-ozone period (6.7 $\mu g/m^3$) as compared to non-event periods (4.6 $\mu g/m^3$). The OC:EC ratio during the June 02 high-ozone event was 7.0—substantially lower than the ratios for the high-ozone period (13.8) and non-event periods (12.0)—suggesting a larger contribution from combustion emissions (higher EC) on this day. The measured species will be used with positive matrix factorization in order to determine sources contributing to fine particulate matter in Zion, IL, with an emphasis on understanding the distribution of primary/secondary and biogenic/anthropogenic sources.

4RA.15

Ice Core Recorded Black Carbon Variations from Muztagh Ata Reveal Kuwait Fires and the Quantitative Evaluation of Source Contribution and Impacts on Glacier Melting. JIAMAO ZHOU, Xuexi Tie, Shuyu Zhao, *Institute of Earth Environment, Chinese Academy of Sciences*

Refractory black carbon (BC) can be transported in the atmosphere from surface to high latitudes and deposited to the ice preserving a history of emissions and atmospheric transport. A yearly resolution BC records from the ice core drilled at Muztagh Ata Mountain are analyzed in order to investigate the BC variations and identify potential source areas by using a global chemical transportation model (MOZART-4). We conclude that the emissions from big Kuwait fires at the beginning of 90s are the dominant source of impurities while the concentrations of BC in the ice core displayed distinct increase by numerical simulation experiments compared with ice core records during the period of Kuwait fires and several pre- and post- years. It suggests that fine BC aerosols from surrounding natural aerosol source regions convectively lifted from the surface boundary layer into the upper troposphere and then integrated with the westerly belt is an effective pathway for BC entering the Muztagh Ata mountains, and increase BC trends in the local glaciers with additional affection by deposition progresses. Quantitative estimation of surrounding sources for the BC concentrations in the Muztagh Ata is firstly carried out by using MOZART-4 model to study the respective transportation pathway and factional contributions. Central Asia is the predominately contribution source region during summer monsoon and South Asia is the largest source during non-monsoon followed emissions from Europe which determined by contemporary emission variation and wet deposition. Furthermore, the albedo reduction and radiative forcing increase caused by black carbon depositing on the surface of snow and ice have been calculated in Muztagh Ata glaciers and BC emissions from the Persian Gult during early 90s had enhanced climate forcing and runoff by over 3 times compared with that of typical normal years. Consequently, emissions in the east part of north hemisphere caused by heavy pollution incidents such as big fires have a tight linkage with BC concentration and deposition trends in the Muztagh Ata. This study provides an important investigation of regional transportation and emissions over east Pamir.

4RA.16

Seasonal Variations of Sahara Dust and Their Impact on the Air Quality over Western Ethiopia- First Cut Results.

SATHEESH M K KUMAR, Amente Dereje Wakgari, *Department of Physics, Wollega University, Nekemte, Ethiopia*

Sahara is the world's largest hot desert lying in low latitude region which spans most of northern Africa (150 to 350 N, 35 0 W to 150 E). Being the second largest arid region after Antarctica in the world and it covers about 9 million square kilometres amounting to 31% land in the African continent, the increasing amount of mineral dust emission from this region plays a pivotal role on the West African air quality and climate (Florence de Longueville et al, 2013). Despite the proximity of the Sahara, virtually no studies related with dust impact on air quality and human health have been initiated in western region of Ethiopia. As Sahara is characterized by periodical outbreaks of dust storms that transport huge amount of mineral dust in the troposphere, it can significantly enhance AOD that is correlated with the aerosol direct radiative forcing (Bart De Paepe et al, 2009, C. Zhao, et al,. 2010). Further, Saharan dust often mix with moist air transported from the Mediterranean build up sporadic clouds which in turn changes the albedo over the western Ethiopian which is lying in a hillock region. This work is a preliminary investigation of air quality variability with the seasonal changes in the direction of air mass over this region with the aid of seasonal changes in the NOAA HYSPLIT back trajectories and the respective changes in the AOD derived from MODIS. This observation further reveals the deterioration of air quality due to the transport of Sahara dust during winter months due to its eastern flow over Ethiopian region. Further, the heavy fog developed in the morning due to the shallow boundary layer across the valley during the winter months contaminated with mineral dust that causes a major health impact in this region with large population. In summer, since the influence of Indian Ocean is more pronounced over this region, the mounting level of moisture induces the development of coarse particles which can vary the weather conditions. The consistent seasonal variations of AOD derived from MODIS over Western African regions ranges from 0.24 to 0.56 reveals the progressive loading of atmospheric aerosols which is in the form different layers also drastically changes the air quality at this region as well (Mamadou Simina Drame et al, 2013). This is the first and preliminary observation from this region and quantification and characterisation of aerosols which are in progress to analyse their prominent role on the variability of air quality in this region.

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Key Words: dust, air quality, radiative forcing, West Africa.

4RA.17

Chemical Composition and Seasonal Variation of PM2.5 in Urban and Rural Regions of the Guanzhong Basin, Northwestern China.

JIN LI, Gehui Wang, Jianjun Li, *Institute of Earth Environment, CAS*

In order to investigate the character of regional air pollution in the Guanzhong Basin, one of the most polluted areas of China, $PM_{2.5}$ samples were collected at Xi'an in July 2016 and a rural site around 100 km northeast of Xi'an in August 2016 and January 2017, and determined for organic carbon (OC), elemental carbon (EC), and inorganic ions. The concentration of $PM_{2.5}$ in summer was 48.88±22.69 $\mu g \cdot m^{-3}$ and 62.60±14.23 $\mu g \cdot m^{-3}$ in urban and rural areas, respectively, and increased to 161.79±87.05 $\mu g \cdot m^{-3}$ in winter in the rural region. At the rural site, concentrations of OC and EC (41.61±22.03 $\mu g \cdot m^{-3}$ and 12.31±5.51 $\mu g \cdot m^{-3}$) in winter were significantly higher than those in summer (6.75±1.81 $\mu g \cdot m^{-3}$ and 3.80±2.27 $\mu g \cdot m^{-3}$), with no significant differences between daytime and nighttime. The correlation of OC and EC was strong (R^2=0.92) in winter, and much weaker (R^2=0.61) in summer, suggesting an enhanced formation of secondary organic aerosols in summer due to the higher temperature and stronger solar radiation. The water-soluble inorganic ions (WSIIs) accounted for 41% and 48% of $PM_{2.5}$ in urban and rural areas during summer, and 41% in the rural area during winter. Secondary inorganic aerosols (SO_4^{2-}, NO_3^-, and NH_4^+) were dominant WSIIs, accounting for 78-91% of total WSIIs. Contributions of SO_4^{2-}, NH_4^+, and K^+ to $PM_{2.5}$ in the rural area were much higher than those in the urban area, indicating the impact of rural agricultural ammonia emissions and biomass burning. In contrast, the higher contribution of NO_3^- and lower SO_4^{2-}/NO_3^- ratio (8.37±5.31 and 2.14±1.32 in rural and urban areas in summer) suggested a more important emission from vehicle exhaust in the urban area. Our results presented detailed information about chemical composition and source contribution of $PM_{2.5}$ in the Guanzhong region and may be helpful for the government to make effective control and management.

4RA.18

Aerosol Characterization in Oujda (Morocco) for the Period 2011-2015. Ibtissam Marsli, MOHAMMED DIOURI, Abdelouahid Tahiri, Djamaleddine Chaabane, *Atmospheric Physic, LME, University of Oujda, Morocco*

This study focus on the data analysis of aerosol optical characteristics: aerosol optical depth, Angstrom coefficient, refraction index, single scattering albedo, radiative forçage and particle size distribution registered by the network AERONET/PHOTONS. Oujda (34.65 °N, 1.89° W) Northeastern of Morocco, 55Km from the Mediterranean Sea. It enjoys a dry climate with a mild winter to cold and rainy and a hot summer marked by the Mediterranean breeze and the influence of the desert air masses coming from the Sahara, called Chergui wind violent, very dry and hot which blows on North Africa and the South of the Mediterranean Sea. Maritime and continental air masses are the dominant daily changes depending on the general weather.

The seasonal cycle of optical thickness at 0.5µm has two periods: the first extends from October to February with low values and small deviations. The second from March to September with relatively high monthly averages which can reach 0.4 with large deviations. These largest values are associated with small values of the Angstrom coefficients characteristic of the presence of mineral dust in summer coming mainly from Southeast. High values of the Angstrom coefficients result mainly from combustion processes (industrial and domestic), road traffic (arrival of emigrants in summer), and construction sites. These results confirm the importance of desert aerosol in summer and less degree in the spring and are consistent with the measurement campaigns carried out early 2000s. The refractive index varies little with an average real part of the order of 1.475 and of the order of 12.3010-3 for the imaginary part. The monthly spectral averages of the single scattering albedo remain high varying between 0.70 and 0.98; the higher values registered in winter where in the absence of clouds the clarity of the sky is dominant. The radiative forcing observed at the top of the atmosphere varies between -20 and +7W/m2, the negative values corresponding to the increase of the reflected flux due to the diffusion of the radiation towards the larger space by the aerosols thus contributing to cooling of the Earth-Atmosphere system and positive values indicate less reflected radiative energy. At the surface, the observed values vary between -140 and -50W/m2 , and are representative of the importance of forward IR scattering of the coarse particle modes characteristic of desert aerosols which cause a decrease in the net flux.

The seasonal average of PSD for the five years seems identical and show larger amplitudes for the coarse mode around an average radius of 2.56µm and with a maximum recorded in summer for which the volume concentrations can reach 0.24µm3/µm2 and confirms the relative influence of Saharan and desert mineral dust advections. The fine mode present a constant at the general average, and remains less important than that of the coarse with an average radius of the order of 0.15µm.

4RA.20

Aerosol Particle Dry Deposition Velocities above Grassland According to the Diameter and the Micrometeorological Parameters: The "V" Curve between 1.5 nm and 1 µm with Three Different Methods. GEOFFREY PELLERIN, Denis Maro, Evelyne Géhin, Philippe Laguionie, Olivier Connan, Didier Hébert, Luc Solier, *IRSN*

Nuclear facilities introduce different types of radionuclides into the atmosphere in the form of gases and aerosols during chronic or accidental releases. These particles may be submitted to atmospheric dispersion, dry and wet deposition. The study of dry deposition based on the dry deposition velocity (dry deposition flux divided by an atmospheric concentration above the substrates) concept is a major issue concerning the impact of radionuclides on the population and the environment. Uncertainties on the dry deposition velocity values of submicronic particles are up to several orders of magnitude discrepancies according to the model used (Petroff et al., 2008). Moreover there is no data for particle diameter under 10 nm. So, the aim of this study is to quantify dry deposition velocity according the particles diameter and the atmospheric stability.

Dry deposition flux can be determinate with different devices. We used 3 different methods to quantify the dry deposition velocities according the particles diameter. (1): For particles around 1.5 nm we studied the dry deposition of free faction of alpha particles of Rn222 decay products by the gradient method (2) For particles between 2.5 nm and 1.2 µm we used the eddy correlation method with a cospectral analysis (Pellerin et al., 2017): the dry deposition flux is determinate thanks to covariance between fluctuations of the vertical wind velocity and fluctuations of the atmospheric aerosol particle concentration during 30-minutes periods at high frequency. The aerosol particle concentration was measured by coupling two Condensation Particles Counters (CPC 3788, TSI, Inc.) for particle sizes between 2.5 and 14 nm (Twin CPC method) and for particle sizes between 7 nm and 1 µm, an Electrical Low Pressure Impactor (ELPI, Dekati, Inc.) was used. The wind 3-component velocity was measured by an ultrasonic anemometer (Young 81000, Inc.). (3) The last method used is the direct deposition of fluorescein particles of 0.6 µm on synthetic grass and the measurement are carrying on by a fluorimeter.

Four experimental campaigns were conducted above a grassland in western France (near Poitiers) april 2015 and September 2016.

The first results of these campaigns show that the particles under 10 nm are influenced only by the mechanical turbulence (link with the friction velocity u*), while the particles over 10 nm are influenced by the mechanical turbulence and the thermic turbulence (link with the sensible heat flux H).

The different results of dry deposition velocities with the three different methods allowed to obtain a “V” curve between 1.5 nm and 1.2 µm. In fact, if we look the curve of dry deposition velocities normalized by friction velocities according to particles diameter and for the four sampling campaign, even if the used different technics, all of the point are consistent. Moreover we can find the theoretical curve shape of dry deposition velocity with the effects of the three dry deposition mechanisms: Brownian diffusion, interception and impaction.

We propose to present the all used methods and devices and then, to describe the results.

4RA.21

Spatial Distributions and Trends in Aerosol Optical Depth (AOD) from CERES-derived and AERONET-measured over South Asia. NEELESH LODHI, Naresh Kumar Soora, Sachchidanand Singh, *ICAR-IARI, New Delhi Inia*

This study presents variability of aerosol over south Asia and its impact on solar radiation using CERES-derived and AERONET-measured observations for long period (~17 years from March 2000 to June 2016). Spatial distributions and trends are shown for CERES-derived parameters like as aerosol optical depth at 550 nm (AOD550), cloud optical depth (COD), photosynthetically active radiation (PAR) and shortwave (SW) fluxes over India. The CERES-derived monthly mean AOD550 values range from ~0.1 to 1.5 and AERONET -measured AOD500 are from 0.03 to 1.6 over India. The highest monthly mean AOD500 (~1.6) is also found at New Delhi (ground-measured Microtops) and lowest AOD500 (~0.03) at Nainital (AERONET -measured). However, both CERES-derived and AERONET -measured spectral AODs are also high (~1.0) at Delhi, Kanpur and Gandhi College during post-monsoon months possibly due to fossil fuel and biomass burning. The highest increasing AOD550 trends are found at Gandhi College (~0.1/decade) and at IIT Khargpur (~0.12/decade) in lower IGP region due to anthropogenic activities. Moderate increasing AOD550 trends (about ~0.05 to 0.06 per decade) are found at Delhi, Kanpur and Pune due to industrialization and urbanization. Increasing trend of CERES-derived AOD550 is found about 0.03/decade at Nainital, but ground-measured AOD500 values are showing decrease trend. The spatial trend range for AOD550 is from ~-0.12 (54%) to ~0.12 (47%), for COD from~-1.2 (23%) to ~0.7 (26%), for PAR from~-4 (6.1%) to ~5 (6%) and for SW from ~-7 (6.1%) to ~15 (6.5%), respectively over India. The negative trend shows decreasing in both fluxes PAR and SW radiation when increasing AOD550 trend over IGP of India.

4RA.22

Measurement of Particle Concentrations in Southern New Hampshire. ANTHONY BARINELLI, Raymond J. Miller, Luke Parkhurst, Chelsea Bitter, Rudra Aryal, *Franklin Pierce University*

This research focuses on the air quality and air pollutant concentration in the southern area of New Hampshire; Jaffrey and Peterborough. Data was gathered for thirteen straight days using the Purple Air II Monitor, which measures various sizes of particulate matter in the air, including dust particles and traffic emissions, using light scattering techniques. The Purple Air II Monitor data was compared with New Hampshire air pollutant concentrations from the New Hampshire Department of Environmental Services database. The data collected regarding air pollutant levels was averaged into three hour intervals for each day and each day's three hours intervals data was averaged with all thirteen days during the same timeframe. The data found a significant amount of air pollutant concentration during high traffic hours in Jaffrey and Peterborough, compared to low traffic hours. The results demonstrate traffic has a significant effect on the concentration of air pollutants people are exposed to, increasing the risk of illness in those who are exposed to high concentrations of traffic emissions and other air pollutants.

*This research was supported by Franklin Pierce University under faculty funding.

4RA.23

Use of Geostationary Satellite Data for AOD Retrieval over India for Air Quality Assessment. RASMA K., Ratish Menon, Harish Gadhavi, Virendra Sethi, *Centre for Environmental Science and Engineering, IIT Bombay*

Satellite AOD retrieval has been reported to be used for ground level air quality assessment. The acceptability of a specific AOD/satellite product varies from region to region. The launch of TERRA and AQUA polar orbiting satellites with sensors such as MODIS, intended for air quality monitoring, have showed promising results over some parts of the world. Further, AOD products from geostationary satellites have also been found to be useful over US, Europe and Japan. There are limited studies for AOD products for geostationary satellites over India. An AOD product from INSAT 3D Imager was studied by comparison against the data from AERONET. The present study investigates the validation and improvements required for application of INSAT data towards air quality assessment over India.

Key words: AOD, Geostationary, AERONET, air quality

4RA.24

Atmospheric Nanocluster Aerosol Emitted from Road Traffic. HEINO KUULUVAINEN, Topi Rönkkö, Panu Karjalainen, Jorma Keskinen, Risto Hillamo, Jarkko Niemi, Liisa Pirjola, Hilkka Timonen, Sanna Saarikoski, Erkka Saukko, Anssi Järvinen, Henna Silvennoinen, Antti Rostedt, Miska Olin, Jaakko Yli-Ojanperä, Pekka Nousiainen, Anu Kousa, Miikka Dal Maso, *Tampere University of Technology, Tampere, Finland*

Traffic is a significant source of atmospheric aerosol particles. Because of their small size and complicated chemical and physical characteristics, atmospheric particles emitted from traffic pose a significant risk to human health and contribute to anthropogenic forcing of climate. Previous research has established that vehicles emit primary aerosol particles and contribute to secondary aerosol particle formation by emitting aerosol precursors. Our recent studies have extended the characterization of traffic emission to cover the smallest particles of traffic environments, referred as nanocluster aerosol (NCA), i.e. the particles in a size range of 1.3–3.0 nm. In the publication by Rönkkö et al. (2017), we reported the significant presence of traffic-originated NCA particles in the vicinity of traffic, determined the emission factors for the NCA, and evaluated its global importance. Our findings demonstrate that, in urban air, extremely small particles form a significant fraction of the total particle number and are a direct result of road traffic emissions. Thus, our findings also imply that an atmospheric nucleation process is not necessary for the formation of a large number of particles in urban areas.

Concentrations and fractions of NCA were measured in three experiments covering a wide range of urban environments. Stationary measurements were carried out at a roadside environment next to a major road in a semiurban area and in an urban street canyon in Helsinki, Finland. In addition, a mobile laboratory was used for a long-distance on-road study through Western Europe. These measurements were supported by experiments in an engine laboratory where the particle emissions of a modern heavy-duty diesel engine were measured at three different engine load conditions. In the engine laboratory experiments, the exhaust was sampled using a partial flow sampling and dilution system previously proved to mimic the real-world exhaust nanoparticle formation. In all the experiments, the NCA concentrations were measured by using a particle size magnifier (PSM, Airmodus Ltd) together with condensation particle counters (CPC). Also carbon dioxide (CO_2) concentrations were measured parallel with the NCA concentrations in order to determine emission factors for the NCA.

In the semiurban roadside environment, the NCA represented a fraction of 20–54% of the total particle concentration in ambient air. The observed NCA concentrations and fractions were depended on the diurnal pattern of traffic and on the wind direction. The emission factors of NCA for traffic were $2.4\cdot10^{15}$ (kg·fuel)$^{-1}$ in the roadside environment, $2.6\cdot10^{15}$ (kg·fuel)$^{-1}$ in the street canyon, and $2.9\cdot10^{15}$ (kg·fuel)$^{-1}$ in the on-road study. However, the emissions were not associated with all vehicles and all driving conditions. In the engine laboratory experiments, the emission factors of exhaust NCA varied from a relatively low value of $1.6\cdot10^{12}$ (kg·fuel)$^{-1}$ to a high value of $4.3\cdot10^{15}$ (kg·fuel)$^{-1}$ depending on the engine load. The high fractions of NCA observed in urban areas indicate that these small particles may have a significant effect on human health and global climate. The determined emission factors showed that the NCA is directly emitted from road traffic and, by using these emission factors, its contribution can be estimated on a global scale.

Acknowledgements

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4RA.25

Intensive Campaign Measurements in South of Romania. CRISTINA MARIN, Luminita Marmureanu, Simona Andrei, Livio Belegante, Alexandru Dandocsi, *National Institute of R&D for Optoelecttronics, UPB*

The uncertainty in deriving the radiative forcing of the aerosols is originating in insufficient understanding of secondary organic aerosol formation and the aerosol-cloud interaction (IPCC, 2013). The complex atmospheric interactions, the night time and day time chemistry that intervene in aerosol formation represent a challenging task even in nowadays.

The intensive campaigns represent a proper method to extensively characterize the atmospheric physical and chemical processes. The results obtained in AROMAT (Airborne Romanian Measurements of Aerosols and Trace gases) campaign held in Bucharest, in 2016, are presented in this study. AROMAT was supported by ESA in the framework of its Copernicus Earth Observation programme and was a preparatory Cal/Val Campaign. The main objectives were to test newly developed instruments for airborne measurements and to prepare the validation programme of the future atmospheric satellites. The measurements took place in two sites in Romania, visible from the Ozone Monitoring Instrument satellite as important NO2 hotspots (Tg. Jiu Valley where is located the Turceni power plant and Bucharest-the capital of Romania).

In this study are presented the results obtained in the last part of the second AROMAT Campaign, the aerosols and gases evolutions being described for the entire one-week intensive campaign, highlighting the main sources present in the South part of Romania.

In order to study the aerosols and gases variability, the measurement strategy involved simultaneous and collocated active, passive remote sensing and in-situ measurements. A comprehensive "picture" of atmospheric structure and composition on vertical and horizontal was obtained through characterization of the planetary boundary height, the aerosol layers derived from Lidar measurements, submicronic nonrefractory aerosol chemical composition (derived from Aerosol Chemical Speciation Monitor), black carbon concentration (from the Aethalometer) and the gases concentration.

For the entire measuring period, the total average mass concentration of submicronic particles is 6.6 µg/m3, from which organic and sulfate have the highest proportion, 46% and 32%, respectively. The black carbon (BC) originated from fossil fuel represented the mainly part, 86% from the total amount of black carbon. BC resulted from fossil fuel and NOx concentration have similar trend, both indicating the traffic emission as the primary source. The low concentrations of BC resulted from biomass burning are in good agreement with the ACSM marker for levoglucosan, f60. The values for f60 are lower than the threshold value for biomass burning aerosols.

During this time, important sources of local anthropogenic and natural long-range transport are identified. Throughout the campaign an important dust intrusion, confirmed by DREAM model, was detected by also passive and active instruments evidencing the presence of non-spherical particles in the upper layers of the atmosphere and an increased Angstrom exponent.

4RA.27

Aerosol Optical Characteristics of Sub Saharan Area. Rajae Meziane, MOHAMMED DIOURI, *Atmospheric Physic, LME, University of Oujda, Morocco*

The present study is devoted to the aerosol optical characterization including PSD, based on data of Aerosol Optical Depths determined with sun photometric measurements for five Sub-Saharan sites, Bujumbura (3.38S, 29.38E), Mongu(15.26S, 23.13E), Gabon(0.20S,11.60E), Namibia(15.15S, 12.17E) and Pretoria(25.75S, 28.28E) and the Atlantic St-Helena Island (15.94S,5.66W) as a reference site. Measurements are made of AERONET/PHOTONS network set up by the Goddard Space Flight Center (NASA, USA) and the Laboratory of Atmospheric Optics (CNRS, France). Sub-Saharan Africa is composed of several types of climate, the main one being that of the tropical savannah that bypasses the equatorial climate. In the South, the subtropical region at first quite humid then tempered until desert.

The seasonal averages of aerosol optical depth at 0.5µm show two categories with low level less of 0.4 near the southern coast as in Mongo, Durban and Pretoria and high level reaching 1.2 for continental sites as Bujumbura and Gabon. Values for St-Helena do not exceed 0.1 outside disturbances observed on August and September. Seasonal averages of single scattering albedo at all wavelengths varies on a large interval (0.4 to 0.98) for continental sites and on a reduced interval (0.8 to 0.95) for the other sites. The radiative forcing observed at the top of the atmosphere varies between -50 and -120W/m2, expressing the increase of the reflected flux contributing to cooling of the Earth-Atmosphere. At the surface, the observed values vary between -200 and -150W/m2, that quantify the local cooling tendency. This tendency is more accentuated reaching -450 W/m2 in Mongu consistent with the large variability of the observed single scattering albedo, and the high surface albedo.

The monthly means of PSD show very higher amplitudes for both coarse and fine modes respectively around an average radius of 5µm and 0.15µm with a maximum recorded in spring for Gabon and Bujumbura expressing an important natural and anthropogenic local pollution. For the other sites, we observe very lower amplitudes around 0.1 and 4 µm respectively for coarse and fine modes that indicate healthy air consistent with the registered AOD values.

4RA.28

Aerosols Measurements Using an Elastic Lidar in Cubatao, Sao Paulo – Brazil. IZABEL DA S. ANDRADE, Elaine Cristina Araújo, Fernanda de M. Macedo, Renata F. da Costa, Eduardo Landulfo, Thais Correa, Maria Helena G.de A. Salani, Roberto Guardani, Maria Lucia G. Guardani, Marcia T. A. Marques, Daniel S. Lopes, *IPEN*

Cubatao is located in state of Sao Paulo, Brazil. This city was considered one of the most polluted places in the world in the late 1970s, being considerate “the valley of death” by the media. The environmental policies were not very strict, favoring industrialization in the region. Nowadays, the state of Sao Paulo has one of the biggest air quality monitoring network in Brazil and more effective environmental policies, however Cubatao still have some issues with air quality. We performed field campaigns with a scanning three-wavelength elastic LIDAR (Light Detection and Ranging), which is a remote sensing technique, with the objective to identify and measure the aerosols emissions in an industrial area. The obtained results demonstrate the aerosol concentration over the study area, the LIDAR technique also helps to identify places that emitted aerosols to atmosphere.

4RA.29

Single Scattering Albedo in Coastal Cities. Azhare El Khabbouti, MOHAMMED DIOURI, *Atmospheric Physic, LME, University of Oujda, Morocco*

Global demographics continue to grow with a human flow increasingly geared towards coastal cities with a strong interest in heat, visibility and air quality. In this study, we analyse PSD, single scattering albedo and induced radiative forcing. These quantities are determined from measurements of the optical thicknesses of the AERONET / PHOTONS network for a sample of coastal sites of great importance at the human activity level composed of Dakar (14.39N, 16.95W), Hong Kong (22.30N, 114 .17E) and Karachi (24.87N, 67.03E) compared with lower activity ones such as Monterey (36.59N, 121.85W) and Santa Monica (34.01N, 118.47W).

The monthly means of PSD show very higher amplitudes of the order of coarse modes and with less degree for fine modes respectively around an average radius of 2.6µm and 0.16µm with a maximum recorded in summer for Karachi, Dakar and Hong Kong expressing an important anthropogenic and maritime mixture, which constitute the main local pollution. For the other sites, we observe very lower amplitudes about 0.04 around the same median radius that indicate healthy air consistent with the registered AOD values.

The monthly averages of single scattering albedo are between 0.8 and 0.97 with the same trend for visible (440 nm) and infrared (1020 nm) for all sites, and with a value close to 1 for the case of Hong Kong. This implies a very important power of Mie diffusion in coherence with the radiative forcing registered. The seasonal averages of radiative forcing observed at sites with a loaded atmosphere are of the order of -67,09 W/m2 at the surface and -28.82 W/m2 at the top of the atmosphere. While for Monterey and Santa Monica, the values are close to zero at the top of the atmosphere and at the surface, thus reflecting the state of radiative equilibrium characteristic of an aerosol-free atmosphere.

4RA.30

Particulate and Gaseous Emissions from Brake Wear: The Eco-brake Project. FULVIO AMATO, Eleonora Conca, Mery Malandrino, Elio Padoan, Apostolos Salmatonidis, Florence Vivier, Agusti Sin, Jana Kukutschová, *Spanish National Research Council (CSIC)*

Due to the strict regulation of vehicle exhaust emissions in the last two decades, about half of road traffic PM emissions are nowadays composed by non-exhaust particles from brake and tire wear and road dust resuspension. The brake wear emissions are poorly understood due to the large variety of chemical composition of brake pads, emission rates and a standardized method for their measurement. The ECO-BRAKE project aims at estimating emission rates for total PM and its components from conventional and innovative (Cu-free and Sb-free) brake pads, including Semi-metallic, low metallic, non-asbesto organic (NAO) and with different types of binder. Several bench tests were performed in a brake dynamometer simulating the emission rates in the AK Master driving cycle. Particle number and mass size distribution were monitored by means of ELPI+ (Dekati), OPS and Nanoscan (TSI). Size resolved components mass and emission rates were obtained by means of DLPI (Dekati) sampler and subsequent ICP-AES and ICP-MS analysis of particles collected on aluminum foils. Other monitored parameters were absorption CO, and CO2.

5AC.1

Global Survey of Submicron Aerosol Acidity (pH). BENJAMIN A. NAULT, Pedro Campuzano-Jost, Douglas Day, Weiwei Hu, Brett Palm, Jason Schroder, Roya Bahreini, Joost de Gouw, Huisheng Bian, Jack Kodros, Simon Clegg, John Crounse, Jack Dibb, Paul Wennberg, Felipe Lopez-Hilfiker, Eloise Marais, Ann M. Middlebrook, J. Andrew Neuman, John Nowak, Jeffrey R. Pierce, James Roberts, Joel A. Thornton, Patrick Veres, Jose-Luis Jimenez, et al., *University of Colorado-Boulder*

Aerosol acidity (H^+, often expressed as "pH" defined in various ways) is an important property that influences uptake and partitioning of gases, and homogeneous and surface aqueous reactions of key inorganic and organic compounds. As there is currently no rapid method to directly measure ambient aerosol acidity, a thermodynamic model, constrained by both inorganic aerosol species (e.g., NH_4, NO_3, SO_4, Cl) and at least one inorganic gas (HNO_3, NH_3, or HCl), is used to provide reliable estimates of aerosol acidity. In this study, we calculated submicron (smaller than 1 µm) aerosol pH from the NASA ATom, "pole-to-pole" series of aircraft campaigns that cover both the Pacific and Atlantic ocean basins in 4 different seasons. The E-AIM thermodynamic model was used with measurements by an Aerodyne high-resolution time-of-flight aerosol-mass-spectrometer (HR-ToF-AMS) of inorganic aerosol species, along with inorganic gas measurements from other mass spectrometers and ion chromatographs. We compare the results with those for the NASA KORUS-AQ, SEAC4RS, DC3, and ARCTAS aircraft campaigns, as well as several ground-based studies, and NOAA and NSF aircraft-based campaigns. We find urban submicron aerosols are typically highly acidic (pH ~ 1 – 2), although the least acidic compared to other environments. Rural/remote continental submicron aerosols are more acidic (pH ~ 0), and remote oceanic ones are the most acidic (pH ~ -1). We compare these results with results from multiple chemical transport models. We find that the aerosol acidity calculated from the measurements are typically 0.5 – 4 pH units lower than the chemical transport models for all locations around the world. This difference would result in dramatic differences in the calculated rates for some important chemical processes. The differences between the chemical transport models and the results calculated from the field observations are currently being investigated, including the impacts of sea salt emissions, meteorology, and atmospheric burden of ammonia and ammonium on aerosol acidity. These results inform the aerosol acidities that should be used in laboratory experiments of submicron aerosol chemistry. Additionally, we demonstrate the importance of accurate aerosol acidity in chemical transport models to ensure these models are properly representing these uptake, partitioning, and homogeneous and surface aqueous reactions of key inorganic and organic compounds.

5AC.2

Factors Affecting Thermodynamic Modeling of Aerosol pH. MICHAEL BATTAGLIA JR., Rodney J. Weber, Athanasios Nenes, Christopher Hennigan, *University of Maryland, Baltimore County*

Aerosol pH is a fundamental property of aqueous particles that affects many chemical and physical processes in the atmosphere. Presently, aerosol scientists lack the ability to directly measure aerosol pH across all ranges of composition and particle sizes. Because of this, the use of aerosol thermodynamic equilibrium models run with gas + aerosol composition inputs has become the most accurate way to predict aerosol pH. Many aerosol thermodynamic models have been developed, but few systematic comparisons of aerosol pH between models have been carried out. This is especially important for aerosol pH since each model possesses unique constraints and limitations on the composition inputs and solution methodology. In this work, we carry out a detailed analysis of aerosol pH computed with three widely used thermodynamic equilibrium models: the Extended Aerosol Inorganics Model (E-AIM), ISORROPIA-II, and AIOMFAC. We focus on pH differences that arise due to factors previously identified as important: the inclusion of aerosol liquid water associated with inorganic and organic constituents, and treatment of non-volatile cations (Ca^{2+}, Mg^{2+}, K^+, Na^+). We add to this analysis the effects of the hydrogen ion (H^+) activity coefficient calculation, and the activity basis (molality, mol fraction, or molar concentration) used to compute pH. The SOAS campaign is used as the basis for comparison since this dataset has been analysed extensively, including analyses of aerosol pH. Overall, we find the activity basis is the most critical factor when comparing different model results, as pH values computed on different bases can lead to inter-model variations of up to several pH units. The other factors are shown to have a cumulative effect on the model prediction of aerosol pH, but at a lesser magnitude than that of inter-model basis consistency.

5AC.3

Aerosol Acidity in the Southeastern United States and Source Impacts on Fine Particle pH. YU QIAN, Armistead G. Russell, *Georgia Institute of Technology*

Aerosol acidity (pH) plays an important role by affecting aerosol formation, particle composition, human health, nutrient bioavailability, etc. This study used species concentration and meteorological data for three monitoring sites from the Southeastern Aerosol Research and Characterization Study (SEARCH) from 2001 to 2013, and thermodynamic model (ISORROPIA-II) to estimate the daily pH trends over that time period. By using the estimated pH time series data, with the help of multiple methods including both simulation and regression, the control factors of pH and the sensitivities of pH to those factors were investigated. Also based on the source apportionment results for the same domain, multiple-linear-regression models were developed to show the impacts of different source categories on fine particle pH. Aerosol pH in SE US kept low (average 2.61) and did not change much over the past decade with the SO_2 emissions reduction, but significant seasonal patterns were observed: high pH during the winter and low pH during the summer, which mainly caused by higher sulfate concentration during the summer. And spatial variations were also observed: higher pH in the urban area and lower pH in the rural area, which were related to higher NH_3 concentration emitted by mobile and biogenic sources (human activities) in the urban area. Model performance was evaluated by comparing estimated and observed NH_3 gas phase partitioning ratio, which confirmed the model performance by showing a good agreement between those two (averaged slope = 0.87, intercept = 0.1 $\mu g/m^3$, $R^2 = 0.65$). Relative humidity and temperature are proved as two strong driven factors of pH, with high RH tend to raise pH and high temperature tend to decrease pH. pH showed largest sensitivity to two species in this study domain: sulfate (-0.11 unit of pH change per 1 $\mu g/m^3$ change of sulfate concentration) and ammonia (+0.10 unit of pH change per 1 $\mu g/m^3$ change of total ammonia concentration). Crustal ions in SE US have little effect on aerosol pH. With strong correlations (average $R^2 = 0.37$), in most cases, models indicated vehicles emissions had the largest positive impact on pH and ammonia bisulfate contributed most negative impact on pH, even though specific results are different for different seasons and locations. Data withholding methods used for evaluating the model performance indicate that the model is trustable ($R^2 = 0.67$).

5AC.4

RH Effect on the Oxidation of α-pinene and the Influence on New Particle Formation. XIAOXIAO LI, Sabrina Chee, Jingkun Jiang, James Smith, *University of California, Irvine*

It is widely observed around the world that the frequency and intensity of new particle formation (NPF) events are reduced during periods of high relative humidity (RH) due to the combination of diminished solar radiation, which leads to low concentrations of precursors such as H_2SO_4 and low volatility organic compounds, together with increased condensation sink that leads to scavenging of precursors and clusters. However, NPF has also been observed in the free troposphere in vicinity of clouds, where RH is typically usually over 90%. NPF has also been observed when RH is above 80% in winter in Hyytiälä, Finland. Despite these observations, most chamber and modelling experiments related to the formation of new particles and its gas-phase precursors have been conducted in low or medium RH. Overall, laboratory, field and modeling studies disagree as to the potential impacts of RH on NPF. The current study focuses on how high RH affects NPF-related gas phase chemistry and new particle formation. These will be explored under a range of RH from 0-95% using a temperature-controlled flow tube and a continuous-flow reaction chamber. Results from flow tube studies show that high RH will increase the generated particle size, decrease particle number concentration and decrease the concentration of low-volatility gas-phase precursors. To identify and quantify the latter, we developed a new inlet for a chemical ionization mass spectrometer (CIMS) that significantly reduces water clustering on reagent ions, the latter of which confounds the interpretation of mass spectra. A comparison between the new CIMS inlet and a commercial inlet based on the design of Eisele and Tanner resulted in identical spectra when measuring precursors to NPF from α-pinene ozonolysis with an enhancement in sensitivity of more than a factor of 10. At RH above 90%, water clusters dominated the reagent ion spectra when using the commercial inlet, whereas for the new CIMS inlet water clustering is eliminated. Detailed chemical composition of low volatility NPF precursors from α-pinene ozonolysis will be presented in addition to measurements of nanoparticle composition using Thermal Desorption Chemical Ionization Mass Spectrometry.

5AC.5

Competing Effects of Water Vapor and Aerosol Liquid Water on the Yield and Molecular Composition of Secondary Organic Aerosols. LAUREN FLEMING, Julia Montoya-Aguilera, Wing-Sy DeRieux, Ying Li, Peng Lin, Alexander Laskin, Julia Laskin, Manabu Shiraiwa, Sergey Nizkorodov, *University of California, Irvine*

Relative humidity (RH) is known to affect the mechanism of gas-phase oxidation of volatile organic compounds (VOCs) that ultimately affects the formation and growth of secondary organic aerosol (SOA). Additionally, high RH results in aerosol liquid water (ALW) associated with an inorganic component, which is known to promote the formation of SOA by oxidizing water-soluble components in the aqueous-phase. These two effects of RH can in many cases counteract each other. For example, it has been shown that the toluene SOA yield decreases with increasing RH in experiments without hygroscopic seed particles and increases with increasing RH in those that use them. The goal of this study was to decouple the gas-phase RH effect and ALW chemistry by investigating the effect of RH and presence of aerosol liquid water (ALW) on the relative yields and chemical composition of various SOA types. In addition, we carried out experiments aimed at understanding the ALW effects on SOA organic compounds over time scales of days, comparable to aging times for SOA particles in the atmosphere. Deliquesced (liquid) or effloresced (solid) ammonium sulfate seeds were prepared in a smog chamber at 90% RH and <5% RH, respectively. The photooxidation of α-pinene or xylene occurred in the presence of conditioned ammonium sulfate seeds at the set RH. In a control set of experiments, no seed was used. A suite of online instruments monitored gas-phase composition (proton transfer reaction time-of-flight mass spectrometer), particle-phase composition (aerosol time-of-flight mass spectrometer), and particle volume concentration (Scanning Mobility Particle Sizer). Filter samples were collected for offline ESI-HRMS and/or DART-MS analysis, which provided molecular composition of SOA. SOA filter samples were aged at 85% RH or 0% RH for 24 hours and their molecular composition was subsequently probed. A "molecular corridor" analysis of the nano-DESI mass spectra resulted in the volatility distributions for SOA produced in the presence and absence of ALW for both SOA samples. Additionally, the SOA's glass transition temperature was estimated in order to predict particle phase state under different atmospheric conditions. The results of this study underscore the importance of the effect of gaseous and liquid water on the chemical composition and key properties of SOA particles.

5AC.6

Insights into Aqueous-Phase Related Secondary Organic Aerosols via Mass Spectrometers in Winter in Urban Beijing.

JIAN ZHAO, Conghui Xie, Weiqi Xu, Wei Du, Qingqing Wang, Wei Zhou, Pingqing Fu, Douglas Worsnop, Zifa Wang, Yele Sun, *Institute of Atmospheric Physics, CAS*

Haze pollution, characterized by high levels of fine particles (PM2.5, i.e. particulate matters with aerodynamic diameter less than 2.5 micrometers), had become a major concerning in megacities in China. Here, we deployed an HR-ToF-AMS with other collaborated on-line aerosol instruments including a SMPS, a CAPS extinction and an AE33 from 17 December to 30 December 2016 during the Air Pollution and Human Health (APHH)-Beijing winter campaign in an urban site. Overall, submicron aerosol species varied drastically with an average value of 126.65 (+96.22) µg m-3, which is much higher than the historic PM1 mass concentrations obtained in recent years, while the contribution of each species to NR-PM1 did not show large differences since 2010, indicating relatively stable sources of NR-PM1 during winter time in urban Beijing among these years. In addition, six OA components including three POA factors (CCOA, BBOA and COA) and three SOA factors (LO-OOA, aq-OOA and MO-OOA) were identified by PMF analysis. On average, CCOA contributed the most among POA to OA with 18.4% and LO-OOA dominated SOA with 31.3% (of OA). The aqueous phase related OOA (i.e. aq-OOA) was clearly identified during high RH period and correlated well with aerosol liquid water content and sulfate mass concentrations. Furthermore, aq-OOA together with a fog related factor (F-OA) and interstitial OA observed in Fresno, California fell into the same square region in triangle plot (f44 vs. f43), which might could define a specific region for aq-OOA in this plot. Finally, filter samples were off-line analyzed by FIGAERO-I-CIMS for aqueous phase related tracers to investigate its properties and the potential processes.

5AC.7

Oxidation of Polycyclic Aromatic Hydrocarbons in Secondary Organic Aerosol Particles. AMBER KRAMER, Kaitlyn J. Suski, Alla Zelenyuk, Staci L. Simonich, David Bell, *Oregon State University*

Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous environmental pollutants which are transported globally on fine particulate matter (PM2.5). Secondary organic aerosols (SOA) are formed through atmospheric reactions of natural biogenic volatile organic compounds, making up a large fraction of PM2.5. Global SOA particle mass has been shown to be increasing due to anthropogenic activity, and have been shown to trap and transport PAHs. SOA particles consist of highly oxidized organic compounds as well as reactive oxygen species. These reactive oxygen species have the potential to react with other organic components such as PAHs. In controlled laboratory experiments, ozone reacted α-pinene SOA was produced with four individual gas phase PAHs present: phenanthrene, dibenzothiophene, pyrene, and benz(a)anthracene. Particles were monitored for changes in physical characteristics, exposed to ozone, and observed over time. Filters of SOA particles were collected and analyzed using gas chromatography mass spectrometry for PAHs and PAH oxidation products. Oxidation products of the experimental PAHs were observed to be in equal concentrations with the parent compound put into the system. The PAH chemistry was observed to change when particles were exposed to 6-10 ppm ozone, using a potential aerosol mass (PAM) oxidation chamber, as well as when particles were analyzed after sitting undisturbed in the reaction chamber for two hours. Data indicates SOA particles are dynamic with continuing chemical reactions occurring.

5AC.8

Fine Particle pH for Beijing Winter Haze as Inferred from Different Thermodynamic Equilibrium Models. SHAOJIE SONG, Meng Gao, Weiqi Xu, Jingyuan Shao, Guoliang Shi, Shuxiao Wang, Yuxuan Wang, Yele Sun, Michael McElroy, *Harvard University*

pH is an important property of aerosol particles but is difficult to measure directly. Several studies have estimated the pH values for fine particles in North China winter haze using thermodynamic models (i.e., E-AIM and ISORROPIA) and ambient measurements. The reported pH values differ widely, ranging from close to 0 (highly acidic) to as high as 7 (neutral). In order to understand the reason for this discrepancy, we calculated pH values using these models with different assumptions with regard to model inputs and particle phase states. We find that the large discrepancy is due primarily to differences in the model assumptions adopted in previous studies. Calculations using only aerosol phase composition as inputs (i.e., reverse mode) are sensitive to the measurement errors of ionic species and inferred pH values exhibit a bimodal distribution with peaks between −2 and 2 and between 7 and 10. Calculations using total (gas plus aerosol phase) measurements as inputs (i.e., forward mode) are affected much less by the measurement errors, and results are thus superior to those obtained from the reverse mode calculations. Forward mode calculations in this and previous studies collectively indicate a moderately acidic condition (pH from about 4 to about 5) for fine particles in North China winter haze, indicating further that ammonia plays an important role in determining this property. The differences in pH predicted by the forward mode E-AIM and ISORROPIA calculations may be attributed mainly to differences in estimates of activity coefficients for hydrogen ions. The phase state assumed, which can be either stable (solid plus liquid) or metastable (only liquid), does not significantly impact pH predictions of ISORROPIA.

5AM.1

Linked Response of Aerosol Acidity and Ammonia to SO2 and NOx Emissions Reductions in the US. ABIOLA LAWAL, Xinbei Guan, Cong Liu, Lucas Henneman, Vasudha Bhogineni, Rodney J. Weber, Athanasios Nenes, Armistead G. Russell, *Georgia Institute of Technology*

Reductions in sulfur (SO_2) and nitrogen oxides (NO_x) emissions have led to considerable improvements in air quality such as lower particulate matter ($PM_{2.5}$) concentrations. However, similar responses in aerosol acidity have not been observed. Aerosol acidity is an important characteristic of particulate matter ($PM_{2.5}$) that has far wide-reaching implications in atmospheric heterogeneous chemistry, biogeochemical cycles, climate forcing and adverse health effects. Studying the impact of the reduction of SO_2 and NO_x emissions, both of which can ultimately constitute a large portion of inorganic aerosol mass fraction, is important to understanding the environmental impacts of future emissions reductions on acidity. Previous spatially limited studies have shown that effects of these precursor emission reductions have had minimal impact on aerosol acidity[1]. Other studies involving a thermodynamic analysis into the neutralizing effectiveness of ammonia (NH_3(g)) on aerosols have shown limited impact of high ammonium concentrations on aerosol acidity[2]. This study expounds upon previous aerosol acidity analysis by conducting a longer temporal and wider spatial study over the continental United States using data from three nationwide ambient concentration networks; the Ammonia Monitoring Network (AMoN), the Clean Air Status and Trends network (CASTNET) and the Southeastern Aerosol Research and Characterization Network (SEARCH) together with a chemical transport model (CMAQ). Further, as aerosol pH is not readily measured, the aerosol thermodynamic model, ISORROPIA II is utilized here to characterize aerosol pH. Results of the study show that aerosol acidity has not responded to nationwide reductions in SO_2 and NO_x, with all observed increases yielding changes in pH of less than 1 unit over varying periods of time. Additional results also show no significant changes in particulate nitrate or atmospheric gaseous ammonia concentrations in response to these reductions. In effect, our study finds nationally, what has been reported for the southeast US[1]; the significant emission reductions in SO_2, NO_x did not significantly impact aerosol acidity. What are the implications of these findings? Maybe a more important question is when, if ever, will the aerosol system become more sensitive or respond differently to these emission reductions.

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5AM.2

Improving SOA Formation in the Source-oriented WRF/Chem Model (SOWC) in Southeast US and the Air Quality and Climate Impacts. HONGLIANG ZHANG, Anikender Kumar, Michael Kleeman, *Louisiana State University*

Aerosols from natural and anthropogenic sources could affect climate by directly absorbing and scattering radiation and indirectly acting as cloud condensation nuclei (CCN). Key features affecting aerosols’ radiative forcing ability such as the primary source origins, differential secondary formation coatings, and mixing state are not well represented in current air quality and climate models. The source-oriented WRF/Chem model (SOWC) tracks particles from different sources separately and has the ability to better predict the aerosol-meteorology-climate interactions. This study, new secondary organic aerosol (SOA) formation pathways (the aging process, aerosol surface uptake and effect of vapor wall loss) are incorporated in the SOWC to investigate the climate effects in Southeast US. Summer 2013 is selected to take advantage of the extensive measurements from field campaigns. The Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System is used to generate source-oriented anthropogenic emissions from the National Emissions Inventory (NEI) 2011. The increase of SOA predictions from each improvement will be quantified and the feedbacks of aerosols to meteorology and climate will be estimated. The results of this project would also encourage the scientific community to include these features in global climate models for long term simulations to reevaluate the past and predict the future.

5AM.3

Improved Prediction of Aerosol Optical and Chemical properties over the Indian Subcontinent from Constrained Aerosol Simulation.

Bharath Kumar, SHUBHA VERMA, Olivier Boucher, Rong Wang, *Indian Institute of Technology Kharagpur*

Role of aerosols in influencing the hydrological cycle is evidenced through studies with aerosol-chemistry-climate models. These studies are required specifically for the Indian subcontinent, as monsoon precipitation being a crucial element of economic growth in India. However, a large divergence between simulated and observed aerosol distribution over the Indian region limits the accuracy in prediction ability of aerosol-climate interactions over the region. This divergence is typically large over the Indo-Gangetic plain, where the atmosphere is observed laden with a high pollutant level of aerosol load. Due to the inclusion of various complex physical-chemical atmospheric and aerosol processes in aerosol-chemistry-climate models, in conjunction with inherent uncertainty in inputs to the model, e.g. aerosol emissions and their properties, a systematic approach is, therefore, required to improve the prediction of aerosols.

With the aim of obtaining a better concurrence between model estimates and observations of atmospheric aerosol chemical constituents and predicting their spatial distribution as consistently as possible, we performed a free running aerosol simulation (freesimu) in a general circulation model (GCM), and further constrained the simulated with the observed aerosol optical depth (AOD). Constrained aerosol simulations are used to establish an alternate approach for estimating the atmospheric concentration by surpassing the error induced specifically due to emissions in source regions which prevails in case of the free running aerosol simulations. The present study was carried out during the pre-monsoon season and for the Tigerz experiment which was conducted at stations over the Indo-Gangetic plain (IGP) and the Himalayan foot-hills in northern India. Our formulation of the constrained aerosol simulation (constrsimu) was based upon an identification of the freesimu with the most consistent estimates of aerosol characteristic among the three freesimu (differing in the source of emissions and resolution) carried out in the GCM of Laboratoire de Météorologie Dynamique (LMD-ZT GCM).

Estimates from constrsimu revealed a good concurrence with the observed counterparts. Black carbon (BC), organic carbon (OC), and sulfate-other water soluble (Sul-ows) constituents estimated from constrsimu amounted to 70%–100% compared to that from freesimu being 20%–50% of their measured counterparts. Also, a good agreement between constrsimu estimated aerosol constituents and the respective observations confirmed the postulation of our formulation that the lack of anthropogenic emissions in aerosol simulation in GCM-indemiss being the primary reason for a large discrepancy between model and observations over the mainland India. Estimates from constrsimu were further used to examine the pattern of the distribution of pre-monsoon mean of aerosol species optical depth and concentration over the Indian subcontinent. Among the aerosol constituents, the pre-monsoon mean of dust concentration from constrsimu was considerably high over most of the Indian subcontinent, the anthropogenic aerosol constituents were, however, specifically predominant over the IGP. While the high value of observed AOD was found being mainly due to dust (>0.3) over the northern–northwestern IGP, it was due to Sul-ows (as high as 0.4) over the eastern IGP, eastern coastline, and the Bay of Bengal.

Improved prediction of aerosol constituents as obtained from constrsimu over the Indian subcontinent region gives an insight on prognostic improvement in free running aerosol simulations in the GCM. This information is also useful towards a more realistic estimation of aerosol-induced radiative perturbations and their climatic implications over the region.

5AM.4

Important Role of Ammonia in New Particle Formation in the Earth's Atmosphere. FANGQUN YU, Alexey Nadykto, Gan Luo, Jason Herb, James Schwab, Joseph P. Marto, Junying Sun, Xiaojing Shen, Kirill Nazarenko, Lyudmila Uvarova, *University at Albany*

New particle formation (NPF, or nucleation) is an important source of atmospheric particles and cloud condensation nuclei (CCN), impacting air quality, hydrological cycle, and climate. Ammonia is the most abundant base molecule in the atmosphere, and has been observed to enhance nucleation in a number of laboratory studies. Despite intensive research over the past two decades, questions remain about the role of ammonia in NPF, including the detailed nature of the physico-chemical processes underlying the observed impacts of NH3 on aerosol nucleation rates and properties. Here we employ the thermodynamic data derived from both quantum calculations and experimental measurements to quantify the physio-chemical processes of NH3 nucleation enhancement, and present a comprehensive kinetically-based H2SO4-H2O-NH3 ternary ion-mediated nucleation (TIMN) that explicitly resolves the dependence of nucleation rates on all major controlling parameters. We show that the presence of NH3 lowers the nucleation barriers for neutral, positively charged, and negatively charged clusters differently, as a result of large difference in the binding strength of NH3, H2O, and H2SO4 to small clusters of different charge states. The model reveals the general preference of nucleation on negative ions, the necessity of relatively high [NH3] to initiate nucleation on positive ions, and even higher [NH3] required to achieve neutral nucleation. The predicted dependence of TIMN rates on [NH3], [H2SO4], ionization rates, temperature, and relative humidity agrees well with laboratory measurements. The newly developed TIMN scheme has been implemented into regional and global models (WRF-Chem, GEOS-Chem, and CESM-CAM5), and evaluated against NPF measurements taken at a site in the heavily polluted area around Beijing, China, and another site in the relatively less polluted northeastern region of the US. We show that TIMN schemes reproduce well the observed NPF events and non-events, and ammonia plays an important role in promoting NPF in the lower troposphere. The implications of the results will be discussed.

5AM.5

Aqueous Formation of Low Volatile Organic Compounds using Coupled CMAQ-MCM-CAPRAM. QI YING, Jingyi Li, Jianlin Hu, *Texas A&M University*

Many of the secondary organic aerosol modules in current air quality models assume equilibrium partitioning of semi-volatile organic compounds with an absorbing organic phase. However, water soluble organics have been identified to account for a significant fraction of ambient organic aerosol mass, suggesting that the aqueous phase on aerosols and fog/cloud droplets may have significant contributions to secondary organic aerosol (SOA). In a previous study, the semi-explicit Master Chemical Mechanism (MCM) was incorporated into the Community Multiscale Air Quality (CMAQ) model (i.e. the CMAQ-MCM-SOA model) to study regional SOA formation by gas-to-organic phase partitioning of thousands of semi-volatile organic compounds (VOCs). In this study, a detailed chemical aqueous phase radical mechanism based on CAPRAM 3.0i was coupled with the CMAQ-MCM to predict the regional formation of low volatile oxygenated VOCs (OVOCs) in aerosol and cloud water. The CAPRAM mechanism treats detailed oxidation pathways of 34 oxygenated organic species of two to six carbons (including 5 alcohols, 10 carbonyl compounds, 13 mono- and dicarboxylic acids, 1 ester, 4 polyfunctional compounds and 1 heterocyclic compound) with ~400 model species and ~ 830 reactions. 3D regional simulations will be carried out for the TexAQS 2006 to evaluate the importance of these low volatile OVOCs in SOA predictions in southeast Texas.

5AM.6

Parametrisation of the Multi-Component System: HOM+H2SO4+NH3, Measured by the CERN CLOUD Experiment.

Simone Schuchmann, HAMISH GORDON, Ken Carslaw, Jasper Kirkby, CLOUD Collaboration, *CERN*

Low-volatility vapours in the atmosphere lead to new particle formation (NPF). The change in particle concentrations over the industrial period that results from changing rates of NPF can lead to a radiative forcing of the climate [1]. The most important gases involved in NPF are probably sulphuric acid, ammonia, and highly oxidised organic molecules (HOMs) [2].

Radiative forcing via changes in cloud albedo can be estimated using a global aerosol model. These models are based on parametrisations of ambient and laboratory measurements, and tested against observations of particles in the atmosphere [3]. NPF leads to over half of particle number concentrations at the level of low clouds [4] and is therefore an important variable to constrain.

The CLOUD collaboration has published studies of the nucleation rate $J_{1.7nm}$ for the pure biogenic system with HOMs [5] and for H2SO4+NH3 [2]. Within these reports, parametrisations were presented, that are implemented in the GLOMAP aerosol model. However, ambient data show that there are locations where HOMs, H2SO4 as well as NH3 are present in significant quantities [6]. In addition, recent (unpublished) CLOUD measurements suggest that the interaction of sulphuric acid, ammonia and HOMs leads to different NPF rates compared to a sum of the individual contributions of these molecules to NPF. To study $J_{1.7nm}$ for the multi-component system (HOMs, H2SO4 and NH3), CLOUD has also measured this system for different temperatures, ionisation states and relative humidities between 2015 and 2017. In this contribution, we will present a parametrisation of this multi-component system and compare the results of GLOMAP including this new mechanism to older model versions.

We thank CERN for supporting CLOUD with important technical and financial resources and the PS beam. This research has received additional funding from numerous sources.

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5AM.7

Application of Boosted Regression Trees Technique to Analyse Particle Number Count Concentrations [PNC] at the East Coast of Malaysia. NOOR ZAITUN YAHAYA, Siew Moi Phang, Azizan Abu Samah, Intan Nabila Azman, *Senior Lecturer, Universiti Malaysia Terengganu, Malaysia*

Study on Particle Number Count Concentrations ([PNC]) were conducted at The Institute of Ocean and Earth Sciences (IOES), University Malaya in Bachok, Kelantan, Malaysia, which located approximately 100m from sea edge of the South China Sea at the east coast of the Peninsular Malaysia.

The study focused to understand particle patterns, temporal and relationship between the meteorological factors (wind speed, direction, humidity, temperature and pressure) and gasses that influence the [PNC] in coastal environment. A one-minute data from 6th January to 5th July 2015 (n=259,200) were collected from the IOES station. [PNC] data were obtained by using Particle Counter GRIMM Model EDM180 which built in with 31 channels and located estimated 20 meter above the ground level. [PNC] data were grouped into two, which are fine particles (FPNC) and coarse particles (CPNC), with diameter between 0.265-2.25µm and 2.75-9.25µm respectively. Statistical data analysis was carried out by using a comprehensive statistical software R programming language and its packages.

FPNC were found are more dominant particle in this area,compared to the CPNC with the maximum of FPNC 5,204,079 counts/liter and only 907 counts/liter recorded by CPNC. A resembling pattern was showed throughout the period, which the increasing number of fine particles starting from early May to mid of June, due to the South-West Monsoon effects. Compared to the FPNC, there were decreasing numbers of particle during the North-East Monsoon (January to March). This shows that particles concentrations is influenced mostly by the speed of the wind and from where it blew from (wind direction).

The Boosted Regression Trees (BRT) model was constructed from multiple regression models, and the best iteration of BRT model was performed by optimizing prediction performance. The FPNC and CPNC model were developed with nine variables in three categories namely time system (time in a day, Julian day), meteorological factors (humidity, temperature, pressure, wind speed, wind direction) and gases (SO2, NOx). The BRT algorithm with combination of parameters lr=0.001, tc=5 and nt=10,000 for both [PNC] that achieves minimum predictive error were found best fit the data. The FPNC and CPNC R(R2) values were found to be 0.87 (R2 = 0.75) and 0.85 (R2 = 0.72) respectively, which indicates both observed and model [PNC] were good correlation to each other. The FAC2 values for both [PNC] are 0.81 and 0.76, which are in the recommended range, which is in between 0.5 to 2. The COE values for both [PNC] are 0.56 and 0.54 respectively, which show the models were in a predictive advantage as the value were approaching to 1. In this case, the developed model was within the acceptable value range for predictive evaluation performance. The analysis demonstrates significant variations in FPNC, largely influenced by SO2 (64.12%), prevailing wind direction (11.82%) with the physical strength index, H-Index = 0.097. Meanwhile the other variables show less than 10% influenced with the FPNC. Contradict to FPNC, CPNC largely influenced by wind speed, Julian day and wind direction, which are 29.84%, 22.46% and 22.17% respectively, followed by other parameters which are 10% and less. The H-Index values for CPNC, wind speed and wind direction is 0.219.

BRT model has the ability to identify the most influential variables and rank it in percentage which very useful for planner, designer and policy maker to take into their considerations in their work. The used of a boosting regression trees model in has proven as a statistical tool for predicting of particles at the coastal environment specifically and for other different area in general.

5AM.8

Understanding Significant Variations of Particle Formation and Number Concentration from Surface to the Upper Troposphere over the Central Pacific Ocean. GAN LUO, Fangqun Yu, Charles Brock, Agnieszka Kupc, Christina Williamson, *The State University of New York at Albany*

Aerosol impacts significantly on cloud properties by serving as cloud condensation nuclei (CCN). The sources of CCN over remote oceans and key controlling parameters remain to be understood. Significant variations of particle formation and number concentration from 0.2 to 12 km altitude over the Central Pacific Ocean area were observed during the ATom first deployment (ATom-1, Aug 3rd-9th, 2016). To better understand the key factors controlling particle formation and number concentration from surface to the upper troposphere, a state-of-the-art global chemistry model with sectional advanced particle microphysics package (GEOS-Chem/APM) is employed in this study to simulate particle formation and size distribution evolution. The predicted condensation nuclei larger than 3 nm (CN3) and other variables along ATom-1 NASA DC-8 tracks are compared with those observed. Major characteristics of CN3 vertical distribution and variation sampled along NASA DC-8 tracks have been captured quite well by GEOS-Chem/APM. CN3 concentrations in the upper troposphere are generally ~10-100 times higher those near the surface and have the highest values over the tropical regions. Our study indicates that particle number concentration is dominated by new particle formation, and key parameters controlling nucleation rates include gas concentrations of sulfur acid and ammonia, temperature, ionization rate, and relative humidity. Precursor gases are transported from surface to the upper troposphere via convection, which result in high sulfur acid gas concentration, nucleation rate, and particle number concentration in the upper troposphere over tropical pacific oceans. The key parameters controlling the growth of new particles and their contribution to CCN at different altitudes over the remote oceans will be discussed.

5AP.1

Understanding the Partitioning of Water and Secondary Organic Matter Using Optically Trapped Single Particles.

STEPHEN INGRAM, Young-Chul Song, David Topping, Simon O'Meara, Jonathan P. Reid, *University of Bristol*

The physicochemical changes experienced by organic aerosol particles undergoing dehydration into the surrounding gas phase can be drastic, with persuasive evidence supporting the existence of a moisture driven glass transition in secondary organic aerosol (SOA) particles.[1]

However, at present, the influence of aerosol in a glassy and ultraviscous state on the partitioning of semi-volatile organic compounds (SVOCs) between the particle and gaseous phases is not clear. Indeed, it may not be governed by equilibrium thermodynamics at all, but instead kinetic factors.

We will begin by presenting recent developments[2] in assessing the evaporation kinetics of water and an SVOC from benchmark ternary aerosol, where both chemical species volatilise in response to a step change in relative humidity (RH).

We find that the contributions to observed size behaviour from each process can be decoupled and treated separately.

Particles are levitated in a standard optical tweezer instrument[3] and sized continuously by analysis of characteristic stimulated peaks in the Raman spectrum. Employing Fickian diffusion modelling4, we extract the compositional dependence of the diffusion constant of water and compare the results to recently published parametrisations in binary aerosol particles.

With reference to a numerical framework developed by Mai et. al.[5], we claim that particle phase diffusivity is also crucial to the timescale and reversibility of SVOC evaporation. Such kinetically limited mass transport manifests as a suppression in the observed vapour pressure above the droplet surface, and could have ramifications for mass loadings and size distributions of organic aerosol, were it to be a common phenomenon under atmospheric conditions.[6]

Moving up in complexity, we also present more recent experiments involving the gas phase ozonolysis of α-pinene in the atmosphere surrounding (dry) saccharide or inorganic particles. Oxidation products of varying volatility are produced which condense onto the surface of the seed particle. The volatility these compounds are then estimated from the size response of the organic shell once the gas phase chemistry is stopped.

It is observed that, under dry conditions, particle phase diffusion of organics is completely arrested: only the outermost layers of SVOC partition back into the gas phase, consistent with a recently proposed non-equilibrium adsorption model of particle growth[7]. Conversely, under humid conditions, equilibrium is approached and a distribution of organics are observed to volatilise without impedance.

By cycling the RH within the optical trap in this way, it is also possible to homogenise and re-vitrify the resultant droplet, encasing the organic mass in a nonvolatile, glassy matrix at a range of water activities. This allows the effect of different particle morphologies (core-shell vs homogeneous) on the kinetics of gas-particle partitioning to be studied.

These data provide insights that can improve the representation of SOA phase state, hygroscopic response and organic partitioning, potentially refining our ability to predict the evolution of organic mass in, for example, regional transport models.

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5AP.2

Growth of Atmospheric Clusters by Organic Vapors: Resolving the Growth Mechanism. JENNI KONTKANEN, Tinja Olenius, Markku Kulmala, Ilona Riipinen, *University of Helsinki*

New particle formation (NPF) is a significant source of atmospheric aerosol particles. According to current understanding, the key compounds in NPF are sulfuric acid, bases (e.g. ammonia and amines) and oxidized organic compounds. Therefore, there is a need for a robust physical description of NPF involving these compounds. One of the mechanisms suggested to depict this process is the nano-Köhler theory, which describes the activation of inorganic clusters to growth by condensation of a soluble organic vapor. In this work, we use molecular-resolution cluster kinetics simulations to investigate if the nano-Köhler theory is able to describe the growth of atmospheric molecular clusters.
We simulated the time-development of atmospheric cluster concentrations starting from vapor monomers up to clusters with mass diameter of ~3 nm by solving the discrete general dynamic equation for each cluster. The simulated systems involved two model compounds: a quasi-unary sulfuric acid–base mixture and an oxidized organic compound. In most simulations, the properties of a sulfuric acid–dimethylamine mixture and a representative low-volatile organic compound were used for the inorganic and organic vapors. We performed several simulation sets to investigate the effects of the volatilities and concentrations of the organic and inorganic vapors on the dynamics of the cluster population. From the simulated cluster concentrations, we determined the contributions of different vapor monomers and clusters to the growth over selected threshold sizes. We also determined the apparent cluster growth rates (GR) using the method that is applied for measured particle size distributions.
We found that the dominant cluster growth mechanism is determined by the organic vapor saturation ratio (S_{ORG}) and the ratio between organic vapor and sulfuric acid concentrations ($C_{\mathrm{ORG}}/C_{\mathrm{SA}}$). When S_{ORG} = ~4–40 and $C_{\mathrm{ORG}}/C_{\mathrm{SA}}$ = ~10–10000 nano-Köhler type behavior is observed: the organic vapor starts to contribute to the growth after a certain size is reached. With lower S_{ORG} and $C_{\mathrm{ORG}}/C_{\mathrm{SA}}$, sulfuric acid dominates the growth at the studied sizes, while with the larger values the organic compound dominates.
We compared the cluster activation size determined from the simulations to the predictions by the nano-Köhler theory and found that the two values can differ significantly. Thus, the nano-Köhler theory cannot be readily used to determine the cluster activation size. On the other hand, cluster GRs were often observed to start to increase around the activation size determined from the simulations. However, other dynamic processes, such as varying vapor concentrations, can also cause a similar increase in GR.

5AP.3

Effect of Temperature on Evaporation of α-Pinene Secondary Organic Aerosol. ZIJUN LI, Angela Buchholz, Olli-Pekka Tikkanen, Eetu Kari, Liqing Hao, Taina Yli-Juuti, Annele Virtanen, *University of Eastern Finland*

Volatility of secondary organic aerosol (SOA) constituents governs their partitioning between gas and particulate phase. Current studies have reported slower SOA evaporation than expected from Volatility Basis Set (VBS) parametrizations, suggesting considerable impacts from particle-phase diffusion and from condensed phase reactions (e.g. oligomer degradation). Aerosol measurements have revealed that lower temperature can significantly hinder molecular diffusion and suppress oligomer decomposition. Given the importance of these processes on SOA evaporation, investigations on SOA evaporation at low temperature are needed.

Here, evaporation of α-pinene photooxidation (αpinOH) and ozonolysis (αpinO_3) SOA was examined under a range of relative humidity (RH), both at warm (20 °C) and cold temperature (10 °C). Briefly, αpinOH and αpinO_3 SOA was generated using an oxidation flow reactor and then selected by two parallel Nano-DMAs with open loop sheath flow. After that, a sample flow of 80-nm SOA was either led directly to the instruments via a bypass line or fed into two 100-L Residence Time Chambers (RTCs). Short residence time data was obtained by varying the bypass tube length, while intermediate and long residence time data were collected from the RTCs during the filling period and in ~1h intervals after SOA filling, respectively. Aerosol characterization was conducted by a Scanning Mobility Particle Sizer (SMPS) and a High Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS). Size selection, evaporation and size change measurement were conducted in the temperature and RH controlled environment.

Evaporation of α-pinene SOA was hindered at lower temperature. This is consistent with the temperature dependence of saturation vapor pressures, but it may additionally suggest a temperature effect in the diffusion limitations in SOA particle bulk and the degradation of oligomers. Different evaporation behavior was observed for αpinOH and αpinO_3 SOA. This different volatility distribution most likely stems from a change in the particle chemical composition which is not represented by the very similar O:C ratio derived for the two SOA types. In addition, a kinetic-based evaporation model, coupled with Clausius–Clapeyron relation, was employed to reproduce the observed evaporation and derive the enthalpy of vaporization. These simulations showed that the derived enthalpy of vaporization was higher than the typical values assumed (30–40 kJ/mol) in global aerosol models.

5AP.4

Effect of Particle Charge on Aerosol Dynamics in Teflon Environmental Chambers. SOPHIA CHARAN, Weimeng Kong, Richard Flagan, John Seinfeld, *California Institute of Technology*

Data from environmental chambers are instrumental to understanding the chemistry of the atmosphere and aerosol formation. A common experiment in atmospheric chambers involves determination of the secondary organic aerosol (SOA) yield, the ratio of the mass of aerosol formed to that of a precursor vapor reacted. Since measurements of the amount of aerosol formed in such an experiment can be carried out only on suspended particles, one must account for particles deposited onto the chamber walls throughout the duration of an experiment to obtain an accurate assessment of SOA yield. The effects of particle charge on the aerosol dynamics within a chamber have long been a source of concern.

Here, we provide a procedure for diagnosing the extent to which particle charge contributes to particle dynamics within an environmental chamber. By tracking the preferential deposition of positively charged particles; by comparing experiments carried out under standard, humid, and highly statically charged conditions; and by performing two-parameter optimizations for the chamber eddy-diffusion coefficient and the average magnitude of the electric field, the effect of charge on the rate of particle wall deposition is isolated. A combined experimental and computational method is also developed for determining values for the eddy-diffusion coefficient and the average magnitude of the electric field within a FEP Teflon chamber. To fully account for the effects of charge on particle dynamics, studies of the effect of air ion concentration on the rate of particle coagulation over a typical experiment are performed and demonstrate, in general, that particle charge is negligible for characteristic chamber ion concentrations. Whereas the effect of particle charge on aerosol dynamics in an environmental chamber must be addressed for each specific chamber, we demonstrate experimentally that for the Caltech Environmental Chamber, charge effects on the rate of particle wall deposition are negligible.

5AP.5

Formation and Evaporation Kinetics of Organic Aerosol from Oxidation of Precursor Mixtures by the Nitrate Radical.

THOMAS BERKEMEIER, Masayuki Takeuchi, Gamze Eris, Michael Walker, Brent Williams, Nga Lee Ng, *Georgia Institute of Technology*

Formation of Secondary Organic Aerosol (SOA) was investigated at the Georgia Tech Environmental Chamber (GTEC) facility from separate, simultaneous and sequential oxidations of the precursors α-pinene and limonene with the nitrate radical (NO3).

For the detailed characterization of nitrated and non-nitrated reaction products in the gas and particle phases, GTEC was equipped with a High-Resolution Time-of-Flight Chemical Ionization Mass Spectrometer (HR-ToF-CIMS) coupled with a Filter Inlet for Gases and AEROsols (FIGAERO) as well as a HR-ToF-MS with the Volatility and Polarity Separator (VAPS)[1]. Aerosol formation was initiated at low temperatures of 5 °C and evaporation of product species monitored during step-wise heating to 42 °C. α-pinene and limonene SOA showed distinct evaporation patterns upon increase in chamber temperature.

The measurement data is analyzed using a novel kinetic modelling approach that utilizes a kinetic multi-layer model to describe the coupling of mass transport and chemical reactions in complex multiphase reaction systems. Special attention was given to gas-phase chemistry, vapor wall loss, diffusion in the particle bulk and temperature-dependent gas-particle partitioning of reaction products. The model simulations, along with FIGAERO-CIMS and VAPS-MS data, allow for distinction of the volatility distributions of nitrated and non-nitrated reaction products. We present evidence for kinetic limitations in the evaporation of organic material and a phase transition during the heating process. A semi-explicit chemical mechanism is presented that represents the experimental data and simplifies the Master Chemical Mechanism (MCM)[2] for the use in complex modelling applications. The chemical mechanism was generated using the Monte-Carlo Genetic Algorithm (MCGA)[3] as global optimization tool.

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5AP.6

Air Ions – the Key in Understating Features in the Surface Atmospheric Electric Field in Relation to Aerosol Processes in the Lower Atmosphere. XUEMENG CHEN, Susana Barbosa, Antti Mäkelä, Jussi Paatero, Veli-Matti Kerminen, Tuukka Petäjä, Markku Kulmala, *University of Helsinki, Finland*

Under fair weather conditions, an electric field in the order of 100-150 Vm^{-1} exists in the Earth's atmosphere (e.g. Tinsley 2008). It was shown based on averaged data that the fair-weather electric field follows an alike diurnal pattern, known as the Carnegie curve, in different measurement locations around the globe (e.g. Harrison 2013). The global variations in thunderstorm activities have been believed to be the cause of this diurnal behaviour in the Carnegie curve (Whipple 1929), following the proposal of the global circuit concept by C. T. R. Wilson (Wilson 1921). In the global circuit concept, the Earth's surface and the ionosphere serve as the two electrodes of a capacitor that gets recharged by lightning activities while leaks under fair weather conditions through the flow of air ions.

Air ions are created by ionising radiation. In the lower atmosphere, air ions interact with aerosol particles. Atmospheric new particle formation, for instance, is one of the main aerosol processes that significantly changes the number size properties of air ions (Kulmala and Kerminen 2008). Air ion properties are altered by aerosol processes whereas the presence of air ions modifies atmospheric electric field. Investigations have been dedicated to understand the relations of air ions to aerosol processes and to atmospheric electric properties, respectively. Yet, there is little effort put in studies characterising the connection between atmospheric electricity and aerosol processes. To understand how atmospheric electric field varies with aerosol processes, air ions, being the medium connecting atmospheric electric properties and aerosol processes, are the paramount parameter.

During June-November, 2017, a measurement campaign was carried out at Hyytiälä SMEAR II station (61°51′N, 24°17′E, 181 m above sea level), which situates in a boreal forest in southern Finland (Hari and Kulmala 2005). We measured atmospheric electric field together with soil radon concentration, atmospheric radioactivity as well as air ion and aerosol number size distributions. The number size distribution data of air ions and aerosol particles is part of the routine measurement system at the station. Moreover, the station also provides access to meteorological parameters to further assist our analysis.

In the presentation, we will focus on features in electric fields in relation to aerosol processes, such as atmospheric new particle formation and wet scavenging. Our preliminary results showed that aerosol formation processes introduce variations in the fair-weather atmospheric electric field that blurs the Carnegie pattern and the washout of airborne radon progeny along with the wet scavenging of aerosol particles can result in a temporary increase in air ion production that modifies atmospheric electric field. With the advantages of our air ion and aerosol measurements, we will elucidate how air ion dynamics are reflected in patterns in the atmospheric electric field in relation to aerosol processes.

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5AP.7

Fragmentation of Ionised Atmospheric Clusters inside a Mass Spectrometer. Monica Passananti, EVGENI ZAPADINSKY, Juha Kangasluoma, Nanna Myllys, Michel Attoui, Hanna Vehkamäki, *University of Helsinki*

The development of Mass Spectrometers (MS) as the Atmospheric Pressure interface Time Of Flight (APi-TOF) and the Chemical Ionisation APi-TOF (CI-APi-TOF) has revolutionised the study of new atmospheric aerosol particle formation. These instruments are able to detect molecules and small clusters, which are involved in the first stages of new particle formation, even at environmental low concentration. However, clusters' binding energies are much weaker compared to molecules; hence they can undergo transformations (fragmentation and/or evaporation) inside a MS easier than molecules. Correct accounting of collision induced cluster fragmentation (CICF) is of vital importance for retrieving the initial cluster distribution obtained in the experiments. Therefore, we decide to carry out a systematic study on the fate of clusters inside the APi-TOF and to develop a model to predict the fragmentation of clusters inside the mass spectrometer.

To investigate the fate of clusters inside the APi-TOF we combined it with a high-resolution Differential Mobility Analyser (DMA). The DMA allows us to measure the clusters size and separate them based on their size. Injecting into the APi-TOF only a mono-mobile size ions distribution it is easier to understand the fate of clusters inside the instrument because only one kind of clusters is studied at a time. We analysed sulphuric acid clusters produced by ElectroSpray Ionisation (ESI) and we focused our study on sulphuric acid trimer fragmentation inside the APi. This latter is made by three vacuum chambers (SSQ, BSQ and PB) where an electric field is applied to guide the ions through the interface. We evaluated the effects of the voltages applied to SSB, BSQ and PB chambers without changing the radio frequencies.

We developed a model to describe the CICF inside the APi. In this model, the charged clusters move through the APi under applied constant and uniform electrical field (defined by the tuning of the instrument). We consider each cluster individually and its trajectory is simulated as a random process. The clusters can be affected by energy transfer at collisions with residual carrier gas molecules and following fragmentation. The probabilities governing the energy transfer and the cluster fragmentation are based on level densities of the clusters and the products of fragmentation calculated by quantum chemical methods. After simulating the trajectory (and the fate) of a big enough number of clusters we calculate the proportion of the fragmented clusters.

The results are very promising, we have observed by the experiments and we confirm it with the simulations that the clusters are mainly fragmented at the interface between the first (SSQ) and second (BSQ) chambers. In this area, the pressure is low enough for the charged clusters to be considerably accelerated under electric field and the same time is still high enough for the clusters to experience collisions with the carrier gas molecules. The collisions induce transferring of the cluster translational energy to rotational and vibrational ones leading to clusters' fragmentation in some cases. We have observed good agreement between the experiments and the model. The development of this model and its validation by laboratory experiments is crucial to correctly interpret the experimental data obtained by APi-TOF instruments for simulating the atmospheric processes. It advances both understanding of the process of the new atmospheric aerosol particles formation and developing of the instruments.

5AP.8

Using Droplet Microfluidic Wells to Study Thermodynamics, Morphology, and Phase of Single Aqueous Aerosol Droplet Systems. Lucy Nandy, CARI DUTCHER, *University of Minnesota, Twin Cities*

Measurements of phase and phase change events in chemically complex aqueous droplets provide valuable information for understanding the dynamic processes in these complex micro-environments. For example, atmospheric aerosol droplets regularly undergo phase changes including liquid-liquid phase separation and crystallization. The phase and mixing state of the aerosol has profound effects on particle morphology, species uptake, equilibrium partitioning, activation to cloud condensation or ice nuclei, and optical properties. Many factors play a role in determining if a droplet will liquid-liquid phase separate, as well as its resulting orientation or morphology of the two phases, such as temperature, relative humidity, and chemical composition of the respective phases. In this work, single atmospheric aerosol droplet chemical mimics are generated in microfluidic channels and stored in passive traps until dehydration to study the influence of relative humidity and water loss on phase behavior. The solution volume of the droplet trapped changes with respect to time, and is calculated by image analysis and correlated with the concentration of the solution to determine water activities at each time interval. The research will help determine mixture liquid-liquid phase separation and efflorescence events of droplets that include presence of other dissolved components and tend to decrease the water activity. The measurements will also be used to parameterize statistical thermodynamic modeling for predictions of thermodynamic properties of aqueous aerosols as a function of relative humidity.

5CA.1

Off-line Analysis of Cloud Water Samples compared to On-line Measurements of Below-Cloud Aerosol Composition: Inferring Cloud Processing Impacts on Organic Aerosol. SARA LANCE, Jie Zhang, Amy Christiansen, Annmarie Carlton, Paul Casson, James Schwab, *ASRC, University at Albany, SUNY*

Aqueous chemical processing within cloud and fog water has been identified as a key process in the formation of secondary organic aerosol (SOA) mass, which is found abundantly throughout the troposphere. Yet, significant uncertainty remains regarding the organic chemical reactions taking place within clouds to produce SOA and the conditions under which those reactions occur.

Routine long-term observations from the Whiteface Mountain (WFM) Research Observatory in upstate NY provide a broad regional view of air quality, where important historical measurements of secondary aerosol formation have been made, focusing on inorganic chemical reactions leading to acid rain deposition. The site is also well-suited for the study of SOA formation within clouds, as the summit of WFM intercepts clouds roughly 50% of the time throughout the summer and the site is deep within the Adirondacks where it is generally undisturbed by local sources. An NSF-funded workshop in Sept 2016 brought together key researchers at WFM to lay out the most pertinent scientific questions relevant to heterogeneous chemistry occurring within fogs and clouds. The workshop culminated in a plan to coordinate chemical analyses of cloud water samples specifically focusing on the organic component. Workshop participants also recommended a pilot study at the WFM to better characterize the meteorological conditions, airflow patterns and clouds intercepting the site for future intensive field operations.

This talk will highlight observations from the 2017 pilot study at WFM, with a focus on off-line chemical analyses of cloud water samples collected at the summit and comparisons to on-line measurements of the below-cloud aerosol composition.

5CA.2

A Study on Light Absorbing Carbon Soot Particles and Their Speciation over Semiarid Region of Indo-Gangetic Basin.

PRATIMA GUPTA, Ashok Jangid, Ranjit Kumar, *DEI, Dayalbagh, Agra, India*

The light absorbing soot particles has high global warming potential after green house gases and affects climate change. The absorbing properties of soot particles are influenced by the nature of surrounding particles. Hence, speciation of carbon soot particles has been done using aethalometer and SEM-EDX over semiarid region of Indo-Gangetic basin. The average mass concentrations of carbon soot particles were found to be 7.4±3.4 μgm^{-3}. The highest soot particle concentration has been seen in winter followed by post-monsoon, summer and monsoon. It may be due to variation in source strength and meteorological conditions. The anthropogenic sources viz., biomass/fossil fuel burning enhances the concentration during winter. The concentration of carbon soot particle at shorter wavelength (UV range) to longer wavelength (IR range) has shown large variations. The monthly spectral variation of soot particles with the fraction of different types of soot particle have been shown at seven wavelengths (370-950 nm). The monthly spectral variation shows the higher concentration of carbon soot particle at 370 nm (UVPM). The variations of aerosol light absorption with wavelength have been extended from the near-ultraviolet to the near infrared. Brown carbon (UVPM370) consists of light absorbing organic matter originates from biomass burning. The daily average of UVPM at 370 nm was 9.3±10.2 µg m^{-3}. The daily average of blue carbon at 440 nm is 7.6±7.8 µg m^{-3}. The blue carbon at 440 nm is a certain classes of organic compounds (such as polycyclic aromatic hydrocarbons). The soot particles at 520 nm are known as green carbon. The daily average of yellow carbon at 590 nm is 7.2±8.3 µg m^{-3}. SEM-EDX analysis revealed the most abundant group of particle of soot carbon is influenced by tobacco smoke. The daily average concentration of RC660 is 6.7±3.7 µg m^{-3}. Hematite mineral dust (Fe_2O_3) has absorption bands in the red region of the spectrum and hence the abundance of this material can increase response of 660 nm channel. Carbon soot particle also gives significant response at IR-II (950 nm). Certain inorganic compounds may show the onset of molecular absorption in the near-infra-red: their presence may increase the apparent result in the 880-nm and 950-nm. Light absorption by aerosols collected in biomass burning smoke varied more strongly with wavelength than aerosols dominated by motor vehicle emissions. The SEM-EDX analysis of carbon soot particles reveals the confirmation of the various elements which are emitted from various sources like burning of biomass and fossil fuel, tobacco smoke, dust particles, sand particles, vehicular emission and mineral dust. This analysis also reveals the confirmation of carbon soot particle associated with the various other elements viz., C, Al, Si, K, Na, F, Ca, Fe, Zn, Cu, etc.

5CA.3

Temperature Matters More than Concentration: CCN-activation of Soot after Exposure to Ozone under Atmospheric Conditions. FRANZ FRIEBEL, Amewu Mensah, *ETH Zürich*

Freshly emitted soot particles are known to be poor cloud condensation nuclei (CCN), but from atmospheric measurements it can be deduced that a significant fraction of soot particles act as CCNs. One process which might contributes to this discrepancy is the heterogeneous oxidation of soot particles. Soot particles have an average atmospheric lifetime of one week. During this time, they are exposed to different aging processes, like oxidation with ozone, which might change how the soot particles interact with water.

The investigation of those processes is an experimentally challenging task, due to the long time span which should be covered. Many studies were conducted in which soot was treated with oxidants at concentrations exceeding the atmospheric average by a factor of 1000. This approach reduces the needed observation time, but in case of ozone it does not consider the non-linear reaction kinetic with soot.

In Winter 2017/18 we conducted a lab campaign at ETH Zurich where we investigated the reaction of ozone with soot particles, under atmospheric conditions. With the CSTR-approach we could observe 100nm size selected soot particle up to 16 h. The particles were exposed to Ozone concentration between 22 and 220 ppb at a temperature range of 5 to 35°C. We measured the CCN-activity at different super saturations between 0.3% to 1.4 %.

It was found, that an increase of the ozone concentration at 25°C, by a factor of 10 (from 22 to 220ppb) lead to a reduction in the activation time by factor 1.8 (from 7h to 3h:50min at 1.0 % super saturation). A temperature increase from 5°C to 35°C at a constant Ozone concentration of 200 ppb lead to an reduction of the activation time by factor 5. Our results indicate, that for an assessment of the cloud formation potential of soot particles the ambient temperature should be considered as much as the ozone concentration.

According to the literature, the reaction kinetics can be best described by the Langmuir-Hinshelwood-mechanism, where the reaction is initiated by the adsorption of an Ozone-monolayer. The speed of the reaction is approximately proportional to concentration of ozone adsorbed on the soot surface, but not to the gas phase concentration. [1] This agrees well with our observations. After exposing soot particle several minutes to different Ozone concentrations, the particle diameter increased by 3% and the particle mass by 20%, but remained almost constant during further exposure. Additionally the ozone concentration in the gas phase had little influence on the activation time.

Based on our temperature experiments we calculated an activation energy of 40 kJ/mol for the time limiting step causing CCN-activation. This value is in accordance with previous findings and indicates that the limiting reaction step for the CCN-activation is a conversion of physisorbed Ozone into organic Ozonides. [2]

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5CA.4

Characterization Of Laser Derivatized Soot Nanostructure Towards Identifying Its Source. MADHU SINGH, Randy Vander Wal, *The Pennsylvania State University*

Soot source identification by characterizing nanostructure of the laser annealed material is based on the premise that soots originating from different combustion sources differ in their nanostructure because of the variation in formation conditions. Conditions of temperature, pressure, fuel, fuel-air-ratio, fuel-air mixing are specific to each source during combustion and differ between sources. Thus, soot produced from different sources will vary to reflect its formation conditions. TEM imaging with the application of image analysis algorithms is used to quantify nanostructure parameters. When sufficiently distinct, the contrasting nanostructure can identify the soot origin. Where similar nanostructure or poorly contrasted nanostructure is observed, subtle differences may be magnified by laser derivatization to enhance lamellae recognition and quantification. Derivatization is a process by which a compound is chemically changed, producing a new compound that has properties amenable to a particular analytical method. Laser derivatization is used here in a similar manner to enhance subtle differences in soot nanostructure upon laser heating. Due to the extremely rapid heating (~ 5 nanoseconds to reach 3700°C) and cooling (microsecond) timescales observed when soot is irradiated with a Q-switched laser pulse, soots anneal incompletely due to apparent kinetic limitations on these timescales. Convolved with these changes are small differences in initial nanostructure and composition that become magnified by the fast heating and rapid quenching.

Source identification is important to pollution receptor models that require knowledge of source contributions at receptor sites. In this study soot samples from known sources are imaged via transmission electron microscopy (TEM) before and after laser heat treatment. Image processing algorithms quantify nanostructure characteristics including fringe length, fringe tortuosity, fringe spacing, stacking and curvature for nascent and laser heated soot. These metrics collectively comprise the identification marker or “fingerprint” for soot. Unknown samples can then be compared against information available from existing samples to identify its source or have a close estimate of what the source may be, both qualitatively and quantitatively. Quantitative comparison for identification uses statistical analyses. By this approach, laser derivatization uses the changed soot nanostructure post laser heat treatment to identify the soot source.

5CA.5

Effects of Uneven Coating on the Absorption Enhancement of Soot Aggregates. WILLIAM HEINSON, Rajan K. Chakrabarty, *Washington University in St. Louis*

Soot Aggregates (SAs) in the atmosphere significantly influence the earth's radiation balance, visibility, and public health. They are formed from high-temperature, incomplete combustion of fossil fuels and biomass burning via diffusion limited cluster-cluster aggregation (DLCA) of spherical monomers. SAs can contain a significant amount of non-refractory compounds coated on to its surface which may enhance the SA's natural light absorptive properties through "lensing" effects. Depending on the strength of the lensing effect, the absorption enhancement can be up to a factor of 3. We studied how the wetting of the coating material onto the SA's affects the absorption enhancement. A Monte-Carlo method was employed to simulate the affinity of the coating materials to wet the SAs. The coated SAs' light absorption properties were then calculated using a discrete dipole approximation (DDA) algorithm. In many climate models, SAs are approximated by an equivalent-mass core-shell spherical model due to the ease of calculating optical properties using Lorentz-Mie theory. Keeping this in mind, we calculated the optical properties of core-shell spheres equivalent in mass to our coated SAs. Comparisons of the core-shell spheres with the coated aggregates showed that the mass absorption cross-sections (MAC) were significantly underestimated in the core-shell approximation when the coating uniformly wetted the SAs. When the coating was not evenly applied to the SAs, the enhancement could be significantly reduced.

5CA.6

Characterization of a Novel Miniature Inverted Burner for Soot Particle Generation. Alireza Moallemi, Mohsen Kazemimanesh, JOEL CORBIN, Gregory Smallwood, Jason S. Olfert, Prem Lobo, *National Research Council Canada*

Carbonaceous particles generated by incomplete combustion can absorb light remarkably well and have a strong climate forcing potential. Additionally, there are substantial concerns about the negative effect of combustion generated carbonaceous particles on public health. The research community employ various types of combustion-based aerosol generators, to study the properties of these particles in laboratories. One such combustion-based aerosol generator is the inverted burner developed by Stipe et al. (2005), which has been proven to be a robust source for soot particle generation and was employed in various studies involving soot particle characterization and instrument calibration. Although this burner was extensively employed in lab-based studies, the relatively large dimensions of the burner make its handling difficult and limit its use in various applications, such as field calibration of aerosol

The miniature inverted burner (“mini-inverted burner”) is a modified design in which the size of the inverted burner has been substantially reduced. The main advantages of this burner are its portability, simplicity, low fuel consumption, and relatively low cost per unit compared to the other commercial portable soot generators. In this study, the general performance of the mini-inverted burner was examined using two different fuels: propane and ethylene, and the tests were performed at various air and fuel flow rates. The capability of the burner to generate particles in a stable and repeatable manner was investigated and its ability to produce particles with a variety of sizes and concentrations was demonstrated. In addition to the particle size distribution, other properties of generated aerosol particles, such as optical properties and the amount of elemental carbon (EC) and organic carbon (OC), were measured. This study shows that the mini-inverted burner is capable of generating particles with a verity of mode sizes (120 nm to 200 nm), and number concentrations ($\sim 5\times10^5$ cm^{-3} to $\sim 3\times10^6$ cm^{-3}). Additionally, in some set-points the elemental to total carbon (EC/TC) ratio of the generated soot particles were found to be larger than 80%, which makes this burner ideal for producing carbonaceous particles with high EC to OC content.

5CA.7

UV-visible Absorption Spectrum of Laboratory-generated Soot Particles. Al Fischer, Taylor Helgestad, Lindsay Renbaum-Wolff, Andrew Lambe, Arthur J. Sedlacek, Christopher Cappa, Andrew Freedman, Timothy Onasch, Paul Davidovits, GEOFFREY SMITH, *University of Georgia*

The absorption by soot particles generated from a methane inverted diffusion flame burner was measured across the UV-visible region of the spectrum. Two cavity ringdown (CRD) laser photoacoustic spectrophotometers (PASs) (405 nm and 532 nm), a lamp/laser PAS (301 nm - 662 nm), and a cavity attenuated phase shift single-scattering albedo monitor (CAPS PMSSA) (630 nm) were employed to measure absorption of suspended particles at a total of 10 different wavelengths. In general, very good correlation between the instruments was found with correlation coefficients, R^2, of at least 0.93. Mass absorption coefficients (MACs) were calculated from measurements of particle mass made using a single particle soot photometer (SP2) and a centrifugal particle mass analyzer (CPMA), resulting in an interpolated value at 550 nm of 7.54 (± 0.43) m^2/g. A power law function with the commonly assumed values of absorption Ångström exponent (AÅE) = 1.0 and $MAC_{550} = 7.5\ m^2/g$ is found to describe the visible part of the spectrum well, but it underestimates UV absorption where the discrepancy is as high as 22%. A power law fit to the entire spectrum yields an AÅE of 1.21 (± 0.08), but a systematic increase in AÅE with decreasing wavelength was observed. It is shown that Mie theory with particles represented by volume-equivalent spheres is not adequate to reproduce the shape of the spectrum regardless of refractive index used. On the other hand, the use of a modified Rayleigh-Debye-Gans approximation with a single, wavelength-independent refractive index is able to do so, though it underestimates MAC values by 25-35% depending on the value of the refractive index used.

5CA.8

Optical Properties and Radiative Forcing of Fractal-like Aggregates of Tar Balls from Wildfire Smoke Plumes. JANARJAN BHANDARI, Swarup China, Giulia Girotto, Barbara Scarnato, Kyle Gorkowski, Allison Aiken, Manvendra Dubey, Claudio Mazzoleni, *Michigan Technological University*

Tar balls (TBs) are carbonaceous spherical particles present in biomass burning smoke. In most studies, based on electron microscopy, TBs are typically reported as individual spheres (mostly ~100-300 nm in diameter). TBs absorb radiation in the UV-visible part of the solar spectrum, and therefore, they are considered a component of brown carbon aerosol. The TB optical properties reported in the literature are highly variable which in turn, make their radiative effects highly uncertain. TBs are typically studied as individual spheres. However, in a recent study, we report an abundance of fractal-like aggregates of TBs from the White-water Baldy complex fire. The optical properties of an aggregate of spheres depend on various factors such as the sphere size, the number of spheres, the refractive index, and the wavelength of the incident light. Therefore, we numerically simulated the optical properties of these aggregates using T-matrix. To determine the significance of the aggregation, we compare the T-matrix results with Lorenz-Mie simulations in two scenarios: 1) Each TB in an aggregate act as an independent sphere, so the cross sections are equivalent to the cross-section of one TB times the total number of TBs present in the aggregate (Mie-N-spheres simulation); this is equivalent to compare an aggregate with its independent components. 2) The entire aggregate is approximated as a volume equivalent single sphere of the same volume as the aggregate (Mie-VER simulation).

We calculated absorption and scattering cross-sections, single scattering albedo and hemispheric upscatter fraction of TBs for each simulation at 550 nm for several different values of indices of refraction including extreme values reported in the literature. To study the impact of number and size of spheres, and wavelength, we performed sensitivity analyses by varying the number of spheres (N = 8, 16 and 32), at five different wavelengths (350 nm, 550 nm, 750 nm, 950 nm and 1150 nm) and for three radii of 50 nm, 75.25 nm and 100 nm. Finally, we estimated the direct radiative forcing (DRF) for each simulation at 550 nm and for high and low surface albedo of 0.8 and 0.06, respectively; assuming an arbitrary TBs optical depth of 0.1.

Taking the T-Matrix as a reference, our simulations show that for single scattering albedo and upscatter fraction, the percent differences between the T-Matrix and Mie-N-spheres are large, up to ~40% and 120%, respectively. Similarly, the differences between the T-Matrix and Mie-VER are up to ~20% and 40%, respectively. The DRF from the T-Matrix differs by more than -1 Wm^{-2} from the Mie-N-spheres, while the DRF for T-Matrix exceeds that of Mie-VER by up to ~ +5 Wm^{-2}, depending on the surface albedo.

Our simulations show that the optical properties and radiative forcing of TB aggregates are considerably different from those of individual TBs and aggregation should be accounted for in radiative transfer calculations.

5CD.1

Synergy between Power Plant and Vehicle Emissions Produce Aerosols Linked to Adverse Cardiovascular Outcomes.

RODNEY J. WEBER, Jenny P.S. Wong, Athanasios Nenes, James Mulholland, Armistead G. Russell, Dongni Ye, Stefanie Ebelt Sarnat, *Georgia Institute of Technology*

Multiple studies have linked adverse health effects to particulate metals. A recent epidemiological study from 1998 to 2013 based on hospital emergency department visits in metropolitan Atlanta found that among a range of PM2.5 components tested, water-soluble iron had the strongest estimated effect on cardiovascular outcomes (risk ratio per 20 ng/m3 increase in water-soluble iron is 1.012, with 95 percent confidence interval of 1.005 to 1.019)[1]. Other shorter term studies have shown that vehicle brake or tire wear and road-dust are a major source of iron in Atlanta[2]. Yet over the period of the epidemiological study, the water-soluble iron concentration time-series closely followed trends in sulfate concentration, not total iron. This included tracking both seasonal trends and dramatic changes in sulfate concentration due to specific emission reductions in coal-fired power plants in the past 10 years. To explain the observed trends, we explore the link between iron, sulfate and water-soluble iron through sulfate's influence on particle pH and liquid water content via model simulations spanning the period of 1998 to 2013. These results demonstrate the importance of atmospheric processing on aerosol toxicity and illustrate an unexpected health benefit of coal fired power plant emission reductions.

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5CD.2

Tissue-Delivered Dose – Not Exposure Concentration – Allows Conversion of Toxicological Studies into Acceptable Human Exposure Limits. OTMAR SCHMID, *Helmholtz Zentrum Munchen, Comprehensive Pneumology Center*

Inhalation toxicology studies with aerosols using animal (*in vivo*) or cell-based *(in vitro*) models of the lung are technologically challenging and typically require advanced aerosol equipment for controlled exposure conditions. In spite of these efforts, conversion of these toxicological data into regulatory relevant recommendations for safe/acceptable human exposure limits is often not possible due to fundamental flaws in aerosol dosimetry.

Frequently, estimated worst case scenarios for human exposure levels are chosen as guidance for toxicological studies and “no-response” at these exposure levels is FALSELY interpreted as indicator for “safe” materials. However, not exposure levels but tissue-/organ-delivered dose is essential for reliably risk assessment. Moreover, the susceptibility of the toxicological model (cell/animal) relative to an equivalent human response has to be assessed carefully. For instance, in vitro cell-based inflammatory responses frequently occur at much higher equivalent dose levels than observed in animal models or humans. All of these issues have to be addressed for reliable risk assessment based on toxicological studies.

In this talk, the key factors linking exposure concentration in toxicological studies to equivalent human exposure concentrations and hence acceptable exposure limits are discussed. Essentially this requires careful consideration of the relationship between exposure concentration (external dose) and tissue-delivered dose (internal dose) which includes aerosol characteristics (size, density and shape) as well as geometry of the exposure system (e.g. lung morphology, geometry of cell exposure chamber), flow conditions (or respiratory conditions) and exposure time. As an example, an overview of currently available aerosol-cell exposure systems and suitable real-time dosimetry methods are presented (e.g. Quartz Crystal Microbalance).

Finally, the most difficult aspect of deriving acceptable exposure levels from toxicological studies is the assessment of model- and response-specific susceptibility factors. This issue will be elucidated by providing typical onset doses for various models and endpoints (cell-based, animal-based, acute/chronic response). These doses will be put into perspective by comparison with real world exposure scenarios in both urban and occupational settings.

This talk highlights the pivotal role of (normalized) tissue-/lung-delivered dose, preferentially in terms of surface area, for reliable risk assessment of inhaled particles. It also highlights important implications for the design of toxicological studies and the development of aerosol technology tailored towards the needs of health-effects studies.

5CD.3

A Novel Weighted Sum Method to Measure Particle Geometric Surface Area in Real-Time. LEO N.Y. CAO, David Y. H. Pui, *University of Minnesota*

This study reports the development of a novel method to measure the aerosol geometric surface area (GSA) concentration with a time resolution of a few seconds. In the method, the commercialized nanoparticle surface area monitor was used and slightly modified. The instrument responses under two different conditions were combined in a weighted sum (WS) fashion to correlate with the aerosol GSA concentration. We present the GSA concentration results and comparisons with well-known SMPS data in both laboratory testing and field measurement. For the laboratory testing, the two methods have a good agreement with a Pearson correlation coefficient of 0.9961; for the field measurements including the indoor and outdoor samplings, both methods agree well with each other. In addition, the new WS method is more stable in the clean indoor air and suitable for outdoor environmental sampling with a slight overestimation (125% of SMPS).

5CD.4

Is the Particle Deposition in a Cell Exposure Facility Comparable to the Lungs? ERWIN KARG, George A. Ferron, Sebastian Oeder, Ralf Zimmermann, *Helmholtz Zentrum München and Rostock University*

Biological endpoints from cell exposure experiments are often taken as indicators for health implications and for the impact of ambient aerosols on the lungs [1, 2]. The advantages of such experiments are their relatively short duration, good repeatability, suitable statistics and cost-effectiveness due to lab-scale facility dimensions. Additionally, with respect to the physical deposition processes, the exposure situation is supposed to be similar to the one in the lungs if particles stay airborne when provided to cells in an air-liquid-interface (ALI) system.

However, geometry and air flow rates in an ALI system deviate considerably from the ones in the human respiratory tract (RT). Computer models for particle deposition were developed [3-5] and are adopted here to mimic the exposure situation, to identify the differences and to characterize the deposition patterns in both ALI and RT. As cells from different parts of the RT can be used in an ALI system, a lung deposition software has to be applied which is able to model the regional deposition in the extra-thoracic, bronchial and alveolar region.

Runs of both ALI and RT model were performed for different particle size distributions, and their output was configured to provide the number of deposited particles per surface area (dose per area, DPA) of exposed cells in both the ALI and the RT regions. The built-in dichotomous human lung structure [6] in the RT model provides number, geometric diameter and length of the airway ducts and therefrom an estimate of their geometric surface area.

Results show the DPA in the ALI being 4-5 orders of magnitude higher than in the alveolar region, as the surface area in the deep RT is extremely high and the inhaled particulate matter is spread out over it. In the bronchial region, however, the DPA of the ALI is found to be higher by a factor of 2-10 only and cumulated deposition is therefore much better comparable. However, hot spots may be present in the airways as lung clearance occurs along defined paths and some locations are not well cleared. Additionally, particles are deposited merely according to aerodynamic processes, and being different in size and composition.

In conclusion, i) due to the high DPA, an ALI exposure experiment mimics the cumulated RT alveolar exposure of days; consequently, the experiment duration can be kept short and concentration can be kept low. And ii) if the DPA in ALI and RT should be comparable, cell lines from the bronchial or extra-thoracic region should be used as biological targets.

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5CD.5

Optimization of DAVID Cell Exposure System for Toxicity Analysis of Nanoparticles at the Air-Liquid Interface. TREVOR TILLY, Ryan Ward, Jiva Luthra, Sarah Robinson, Arantzazu Eiguren Fernandez, Saber Hussain, Tara Sabo-Attwood, John Lednicky, Chang Yu Wu, *University of Florida*

Understanding the health effects associated with the inhalation of nanoparticles is critical for determining the risk they pose during occupational and environmental exposures. The many different types and variations of nanoparticles has made evaluating their toxicity burdensome by *in vivo* methods alone, and resulted in the development of many different in vitro toxicity analyses. Despite this development, the current existing methods of *in vitro* have drawbacks when evaluating occupational and environmental exposures of nanoparticles resulting from their fundamental properties. For instance, the process of collecting nanoparticles from the environment on filters and then later extraction in media for toxicity analysis in the laboratory can greatly alter the properties of the particles directly after emission, and subsequently alter their toxicity outcome. To remedy the incorporation of these particle transformations that can result from sample collection, air-liquid interface (ALI) exposure systems have been developed to deliver nanoparticles from aerosols directly to cells. However, deposition of nanoparticles on cells at the ALI may be skewed to a certain size range of particles because the aerosol methods of thermophoresis and electrostatic precipitation often utilized to increase deposition efficiency in these systems are dependent on particle charge and size. A new cell exposure system known as DAVID, Dosimetric Aerosol *in Vitro* Inhalation Device, was designed to improve the delivery of a broad range of nanoparticles through increased inertial force accomplished by amplifying particles as small as 10 nm to a uniform size of 3 µm by condensing water vapor onto the particle. With this technology, evaluation of the toxicity of nanoparticles was achievable with short exposure times by delivering a concentration of particles that met or exceeded the lowest observed adverse effect level. Custom cell culture supports were fabricated by 3D printing, functionalized by oxygen plasma corona for cell attachment, and sterilized with ethanol and UV. With the current setup, four cell membranes cultured at the ALI can be exposed simultaneously so that statistical analysis can be performed within each exposure trial. First, the delivery of clean air to the cell surface was optimized in DAVID to ensure that the flow rate would not cause adverse effect to the cells by drying them out. A flow rate of 2.1 L/minute/cm^2 was selected based on sampling recommendations, but resulted in a reduction of cell viability by 25% of control. Therefore, the flow rate was reduced to 1.4 L/minute/cm^2 and was found to maintain greater than 97% viability of the cells. The deposition of nanoparticles in DAVID was calibrated and determined to increase linearly with time from an uranine aerosol generated by a Collison nebulizer with a mean particle size of approximately 58 nm. The raw fluorescence of the collected uranine droplets on the membranes was measured and related to a calibration curve to determine the deposition mass concentration. Nanoparticle concentration in the nebulizer and dilution flow rate was directly related to the mass deposition of particles in DAVID, which resulted in a mass deposition ranging from 177 ng/cm^2 to 2.93 µg/cm^2 for exposures up to 20 minutes. Post optimization, the cells were exposed to CeO nanoparticles with mean diameter of 39.5 nm generated by the Collison nebulizer in the laboratory, and the delivered dose was assessed by inductively-coupled plasma mass spectrometry. The viability of the cells after exposure was assessed by lactate dehydrogenase assay (LDH) and related to the deposited dose of particles on the cells. Future studies to determine mechanistic nanoparticle-cell interactions at the ALI are the next step for the DAVID exposure system.

(PA Case No 88ABW-2017-5860, 20 Nov 2017)

5CD.6

Oxidative Potential of Quinones in Simulated Epithelial Lining Fluid Alone and in Combination with Redox-Active Metals. KARSTEN BAUMANN, Marco Wietzoreck, Jake Wilson, Pourya Shahpoury, Steven Lelieveld, Haijie Tong, Ulrich Pöschl, Gerhard Lammel, *Max Planck Institute for Chemistry*

The human health risk posed by reactive oxygen species (ROS) produced from fine particulate matter ($PM_{2.5}$) components in epithelial lining fluid (ELF) of the deep lung is a matter of intense scientific interest (Lakey et al. 2016). In aerobic metabolism, oxidative stress can be exerted by excessive ROS comprised of free radicals such as O_2^-, OH, ROO, RO, and non-radical species such as H_2O_2 and O_3. Upon inhalation, many oxygenated and nitrated polycyclic aromatic hydrocarbons (NOPAHs) in airborne $PM_{2.5}$ may contribute to ROS formation, most effectively quinones, which form O_2^- by reactions involving the semiquinone radical. NOPAHs are found regularly in the ultra-fine fraction of $PM_{2.5}$, and can be emitted by incomplete combustion processes (e.g. from diesel engines and biomass burning) or formed in atmospheric photochemical processes. Quinones are known to trigger and maintain catalytic reaction cycles causing oxidative stress at the cellular level (Bolton et al. 2000). In assays addressing the so-called oxidative potential (OP), which is assumed indicative of ROS formation, different redox-active components of ambient $PM_{2.5}$, such as quinones or transition metals, esp. Cu, Mn, Fe, can cause synergistic or antagonistic effects (Xiong et al. 2017, Yu et al. 2018). However, this chemistry is not well understood yet.

In order to investigate each redox active species' OP individually and in combination, we developed an experimental setup representing extracellular conditions in the deep lung that allows reproducible loading of a simulated ELF, containing antioxidants, electrolytes, surfactants and proteins (Boisa et al. 2014). This SELF was refined by sterile filtration, in order to decrease bacterial impurity. Hydrophobic polystyrene latex (PSL) spheres with nominal 60 nm diameter are used to mimic transport of NOPAHs to the alveolar region. The PSL also enhance atomization of select NOPAH compounds dissolved in a mixture of organic solvent (ACN or DMSO) and ultrapure water. The generated particles are collected by continuously refluxed SELF in a mist chamber, and simultaneously on a quartz filter. Delivery and uptake kinetics of two nitro-PAHs and three oxy-PAHs, have been investigated.

The OP and ROS yield of the differently loaded SELF is determined by means of three acellular assays, in particular H_2O_2 formation (Sigma-Aldrich 2014), DTT depletion (Charrier & Anastasio 2012), and antioxidant depletion (glutathione and ascorbic acid). We present and interpret the results in light of possible synergistic or antagonistic effects. Ongoing modeling (Lakey et al. 2016) may benefit from insights gained.

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5CD.8

A Semi-Automated System for Measuring the Reactive Oxygen Species (ROS) Catalyzed by Ambient Particulate Matter (PM) in a Dithiothreitol (DTT) Assay. HAORAN YU, Joseph Puthussery, Vishal Verma, *University of Illinois Urbana-Champaign*

The oxidative potential of ambient particulate matter (PM), i.e. the ability to generate reactive oxygen species (ROS) in the presence of a biological reductant, has been investigated for a long period of time. In our previous study, we found that dithiothreitol (DTT) could be used to indicate the oxidative potential of PM by measuring both consumption rate of DTT and generation rate of •OH. Although, the measurement of DTT consumption has already been automated, •OH measurement, which is a labor-intensive process, still employs a manual protocol, limiting the number of samples that can be analyzed in a day. To overcome this problem, we are developing a system for analyzing the oxidative potential of PM liquid extracts based on the DTT assay in a semi-automated mode. This system uses DTNB to determine the concentration of DTT, and terephthalate (TPT) to capture the •OH generated from the oxidation of DTT. An automated Kloehn control pump system with sample injection valve is used to automate the protocol. A liquid wavelength capillary cell (LWCC) and a Horiba spectrofluorometer are used for quantifying the DTT and •OH concentration, respectively. The system will be calibrated with pure substances (9,10-phenanthraquinone, PQ and 5-Hydroxy-1,4-naphthoquinone, 5-H-1,4-NQ) as the positive controls, and will be tested for its performance with the real ambient PM samples collected from an urban site. The detection limit, accuracy and precision of the system will be evaluated. The seasonal variability in the oxidative potential of ambient PM measured by this system will also be presented. Finally, we anticipate that system can be coupled to a PM sampling device to monitor the oxidative potential of ambient PM in real-time.

5CM.1
Lower Order Representations of Evolving Particle Size Distributions for Rapid Gas-Particle Mass Transfer Simulations during Electrostatic Precipitation. HEREK CLACK, *University of Michigan*

The range of particle sizes typically present in combustion flue gas complicates predictions of gas-particle mass transfer processes. This complexity is amplified within electrostatic precipitators where particle motion, abundance, and mass transfer characteristics are all size dependent. The present study illustrates the utility of replacing explicit representations of particle size distributions in simulations of electrostatic precipitators with an equivalent loading of monodisperse aerosols of diameter chosen to reproduce the same gas-particle mass transfer characteristics. Computational times are reduced by an order of magnitude using this approach, facilitating future incorporation of multiple particle types or heterogeneous chemical kinetics.

5CM.2

Development of Filter-free Particle Filtration Unit Utilizing Condensational Growth. Taejune Park, Miji Lee, Juwon Pyo, DONGGEUN LEE, *Pusan National University*

The public health impact of particulate matter in ambient air with a size of 2.5 µm or smaller (PM2.5) has been of great concern. It is well known that PM2.5 is much more harmful to human health than coarse particles. To remove PM2.5, most air purifiers on the market have been equipped with a high efficiency particulate air (HEPA) filter. Under the circumstances that generate PM2.5 aerosols at high concentrations such as during indoor cooking or in work places, HEPA-grade filters are neither durable nor applicable because of their high replacement cost. Thus, a large number of cooks and workers are exposed to intensive emissions of PM2.5 without proper filtration. In this paper, we introduce two conceptual designs to remove PM2.5 without HEPA filters. A key idea of the first approach is to use the condensational growth of particles. Once the particles have grown to a few micron, they are much easier to remove because of their increased inertia. Based on this, we developed the first prototype of a filter-free particle filtration unit consisting of an air saturator (equipped with water spray nozzles), a condenser in which humid air is cooled down to a supersaturation state and thereby allows particles to grow by condensation, and a multi-nozzle-impactor assembly for collecting the grown particles downstream of the condenser. We started with a small-scale model, and then demonstrated that a large-scale prototype could remove organic, inorganic, and metallic ultrafine particles with a collection efficiency of larger than 80% at a volume flow rate of 50- 92 L/s.

5CM.3

A Corona Charger System for Improving Particle Filtration Efficiency of Flue Gas Scrubbers and Cyclones in Small Biomass-fired Boilers. HEIKKI SUHONEN, Ari Laitinen, Miika Kortelainen, Arunas Mesceriakovas, Hanna Koponen, Petri Tiitta, Pasi Yli-Pirilä, Jorma Jokiniemi, Olli Sippula, *University of Eastern Finland, Kuopio, Finland*

New flue gas particulate matter filtering technologies are needed due to upcoming new regulations for small and medium -scale biomass combustion appliances in Europe. The Ecodesign directive will affect combustion appliances with a rated heat output of 500 kW or less and the Medium Combustion Plant (MCP) directive boilers of 1-50 MW output. Existing commercial flue gas cleaning techniques are often either too expensive compared to the total costs of small boilers, provide too much pressure loss and maintenance, or are not efficient enough to meet the new regulations. Therefore, new methods for cost-efficient particulate filtering need to be developed. For existing boiler units the utilization of electrical charging of flue gas particles upstream of heat exchangers or in front of existing particulate filters is an interesting low-cost approach to improve the filtration efficiency of particles.

A single needle corona charger (Laitinen et al. 2016), was used together with a pilot-scale condensing heat exchanger (CHX) (Grigonyte et al. 2014) and a cyclone, which were installed into a wood chip fired combustion reactor simulating automatic grate boilers. The single needle corona charger is mechanically simple and can be introduced into the flue gas in existing devices and shielded against contamination, while the CHX and cyclone provide the collection surface and additional cleaning mechanism. The effects of charging temperature and different combustion conditions on the charger performance were investigated by changing the charger position in the combustion reactor and using it with different fuel qualities.

Total particle mass emissions were reduced by >80 % with the combination of charger and CHX while the combination of the charger and cyclone setup was slightly less efficient. Particle number reduction efficiency varied between 30 % and 70 %, because the usage of the corona charger produced a nucleation mode below particle size of 30 nm that was highly dependent on the charging temperature and voltage. Particle mass was measured also from between the charger and CHX, for estimating the reduction efficiency of the CHX alone. PM1 emissions were reduced in the CHX by 30-40 % when particles were not charged and 60-70 % when particles were charged before the CHX. Chemical analysis of the condense water from the CHX support the results as enhanced concentrations of typical components of wood combustion fly ash were also found in the water.

The results indicate that a simple corona charger system can provide a feasible particle filtration system together with a condensing heat exchanger, wet scrubber and/or a cyclone to achieve the upcoming new regulations. The system is best suited for small-scale boilers but can be upscaled by increasing the number of corona chargers.

This work was funded by the European Regional Development Fund, within the Pyreus project.

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5CM.4

Correlation Between Corona Current Distribution and Collection of Sulfuric Acid Aerosol in a Wet Electrostatic Precipitator. YIFAN WANG, Chenghang Zheng, Xuefeng Zhang, Zhengda Yang, Yi Wang, Dawei Duan, Xiang Gao, *Zhejiang University*

The emission standard have become increasingly stringent in recent years as more attention has been given to the sulfuric acid aerosols. Wet electrostatic precipitator (WESP) is typically used to remove sulfuric acid aerosols. However, removing sulfuric acid aerosols with small size and high concentration were less efficient.

Enhancing the electric field intensity and optimizing distribution characteristics of the electric field are the key to improve the collection efficiency of the WESP. However, the current researches mainly focused on the influence of discharge electrode geometry on V-I characteristic. Few researches have been done on the detail current density distribution which comprehensibly reflects electric field.

In this study, detailed current density distribution on the collecting plate were researched. An experimental WESP which the current density of measuring point can be obtained automatically was designed. Twenty-three kinds of discharge electrodes with different needle shape, length, and spacing were used as the experimental discharge electrode. Firstly, V-I characteristic of the experimental discharge electrode were measured. Then, we investigated the circumferential and axial current density distribution using current measuring device. And fractional discharge electrode were tested in sulfuric acid aerosols.

The results show that the effect of sulfuric acid aerosols space charge is significant and causes corona current decrease sharply at high concentration. Reducing the current density at the entrance by 87% in 53.6 mg/m^3 sulfuric acid aerosols. Increasing the needle length and decreasing the spacing of needles can provide higher corona current density. Interestingly, the rotating of discharge electrode almost makes no differences to the V-I characteristic, but the current density distribution changes significantly. The current distribution becomes more uniform and improves the removal performance. Rotating 30° relative to the vertical surface is the best choice under the experiment condition. And we will develop a numerical modeling to verify the effects for the corona current and collection efficiency in barbed electrode.

5CM.5

Exploring the Methods of Enhancing the Particle Charge in ESP. DAWEI DUAN, Chenghang Zheng, Qianyun Chang, Zhengda Yang, Yi Wang, Yifan Wang, Xiang Gao, *Zhejiang University*

Electrostatic precipitator (ESP) is a widely used particle control device for its high efficiency and wide adaptability. The overall mass based collection efficiencies for ESPs exceed 99%. However, results of field measurements have shown that there is a “penetration window” in the submicrometer size ranges, where the collection efficiency is as low as 70～80%.Hence, improving the collection efficiency on the particle of submicrometer size ranges is the key to decrease the emission concentration of ESP. The key to improve the collection efficiency of the particle of submicrometer size ranges is to increase its charge.

Many factors such as ion density, electrical field strength, particle properties, flue gas parameters and so on can affect the particle charge. The current researches mainly focused on the influence of ion density and electrical field strength on particle charging. Few researches have been done on the influence of particle parameters and temperature on the charge of particles. In this study, an experimental ESP was designed to explore the effects of particle properties (particle size, composition, etc.), flue gas parameters and water droplet humidification on particle charge. The temperature can be controlled from 298K to 383K and water droplet concentration can be controlled from 2.0 to 8.8g/m^3. Six kinds of fly ash with different dielectric constant were used as the experimental particle. An electrical low pressure impactor (ELPI$^+$) was used to measure the fractional particle charge.

The results showed that the particle charge increased with the increasing temperature. The charge of particle with the diameter of 1.2μm was enhanced by 25% with the temperature improved from 300K to 363K. In addition, particle charge increased as the dielectric constant increased. Besides, when the particle had a water layer on its surface, the particle charge was much larger than without the water layer. The average charge of particles larger than 0.5 μm was increased by more than 35% with the water droplet concentration of 8.8g/m^3.

5CM.6

Development of Electrodynamic Dust Shield Technology for Solar Energy Applications. BING GUO, Wasim Javed, Benjamin Figgis, *Texas A&M University at Qatar*

In the Middle East and North Africa (MENA) region, efforts of utilizing the abundant supply of solar energy can be significantly hampered by soiling of solar panels or mirrors due to dust accumulation. Electrodynamic dust shield (EDS) is a technology using electrodynamic activation to repel dust particles accumulated on a surface, which has been proposed for mitigation of soiling. In the past two years, we have carried out laboratory experiments and field tests to investigate the feasibility of this technology. In laboratory studies, we have found the dust removal efficiency to be dependent on dust loading, dielectric cover thickness and other factors. The dust removal efficiency may decrease to very low levels when the dust loading is low, or when the EDS is run in the cyclic-operation mode. Our field tests, run in the cyclic-operation mode, have shown that EDS prototypes can maintain a dust removal efficiency of approximately 14%, which in theory could still result in significant soiling mitigation benefits. Our field test of EDS-integrated solar photovoltaic (PV) modules has recently begun, and produced some very interesting results. In this presentation, we will give an overview of these results and discuss research needs in the very near future.

5CM.7

Electro-scavenging of Airborne Particles by Electro Hydrodynamic Atomizer (EHDA) Generated Charged Droplets.

Arshad Khan, Sanjay Singh, B.K. Sapra, Y.S. MAYYA, *Bhabha Atomic Research Centre, Mumbai*

Airborne particulates generated during various processes in conventional or nuclear industries are controlled /removed by filtration systems based on their particle size using cyclone, fabric filters and electrostatic precipitator. Cyclone is useful mainly for particles of few micrometers and above. High Efficiency Particulate Air (HEPA) is also suitable and have an efficiency of 99.97 % for particle of 0.3 µm but they are not very cost effective as they need to be replaced frequently due to dust loading. Electrostatic Precipitator (ESP) on the other hand, is used for fine particles of less than 0.3 µm. Though, electrostatic precipitators do not require filter replacement, they produce ozone as a by-product and collection efficiency is low for size 0.1 – 1.0 µm [1].

Alternatively, electro-scavenging of aerosols using charged particles is an upcoming technology in the area of air cleaning. Its advantage is that it does not give rise to ozone in the ambient environment and does not add to the noise level. Herein, we studied the depletion of lab generated aerosols with EHDA generated high charge (~10^4 elementary charges) droplets and its potential for utilization in air cleaning applications [2].

An EHDA based air cleaning system is designed [3] & fabricated and aerosol scavenging characteristics are studied using smoke and nebulizer generated NaCl aerosols. Both types of aerosols were fully characterised with respect to their number, size and charge distribution. For smoke aerosol, size dependent aerosol collection efficiency showed minima of 20% for particle diameter of 30 nm; increasing to as high as 90% for particle diameter greater than 100 nm. For NaCl aerosols, collection efficiency is almost flat with respect to particle size. The variation is 70% to 90% for the particles more than 200 nm.

The EHDA based cleaning system showed good particle removal efficiency, however a question arises as to whether the removal occurs because of electro-migration of aerosols in the capillary electric field of EHDA or due to scavenging of aerosols by droplets. To confirm this, a comparative aerosol removal study was carried out at applied capillary potentials of 0 V and 4 kV (which is just below the operating voltage of EHDA) and with operating EHDA. The experiment confirms the aerosol removal by interaction of charged droplet with aerosol particles. Results from the current system have been very encouraging for its utilization in air cleaning application.

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5CM.8

High-efficiency Particulate Removal by Photoionization Enhanced Electrostatic Precipitation. TANDEEP CHADHA, Jiaxi Fang, Pratim Biswas, *Applied Particle Technology, LLC*

Over the past several years, indoor air quality has become a matter of increasing concern both due to the presence of non-viable pollutants (particles, volatile organic compounds, and gaseous pollutants) and viable pollutants (bacteria, viruses and mold). The efficiency of current media-based filters is limited to particulate removal and is proportional to the pressure drop across the filter. Electrostatic precipitators (ESPs) are considered a viable alternative to media based filtration technology since they contribute a much lower pressure drop and do not require frequent filter replacement. However, ESPs have a limited removal efficiency especially for ultrafine particulates and are associated with the production of harmful byproducts such as ozone.

In this work, we present the development of a scalable photoionization enhanced electrostatic purification (PE-ESP) technology for high efficiency removal of particulates [1]. A model driven approach was used to design and develop a parallel plate PE-ESP system. Air jet atomization of a KCl solution was used to generate aerosolized particles and the filtration efficiency of the SXC-ESP unit was measured using an optical particle counter (OPC) and a condensation particle counter (CPC).The PE-ESP system shows a 97-99% particulate removal efficiency in the 0.2 to 1 µm size range without the production of any measurable ozone. The efficiency without the photoionization was 50-60% in the same size range. The efficiency predictions from the model match well with the experimental measurements for both a conventional ESP as well as the PE-ESP. Owing to its high efficiency and negligible ozone production, the PE-ESP system has the potential of being used as a replacement for media based filters.

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5IM.1

Scattering Matrices of Single Levitated Particles. ALEXANDRIA JOHNSON, Maria Zawadowicz, Sara Lance, Daniel Cziczo, *MIT*

Suspended particulates are a ubiquitous feature of planetary atmospheres. However, major gaps remain in our understanding of how non-spherical particles scatter and polarize incident radiation. Modeling the highly complex scattering phase functions produced by non-spherical particles is challenging and broad stroke simplification of particulate properties, such as with an oblate spheroid approximation, can lead to large uncertainties in numerical model outputs and satellite retrieval corrections.

With this in mind we aim to directly measure how non-spherical atmospheric particulates interact with radiation through the development of a single particle scatterometer. Our novel instrument consists of a vapor diffusion electrodynamic balance (EDB), used to levitate single particles in a precisely controlled atmospheric environment, coupled with a photomultiplier for the collection of a scattering phase function, or scattered light as a function of angle along the plane of illumination.

Here we will discuss the development of our EDB scatterometer, validation experiments with spherical particles, and preliminary results on non-spherical particles. For spherical validation experiments our results will be compared directly to Mie theory and used to address any biases in our measurements. Although single particle studies allow for the precise control of a sample and its environment, their relevance to atmospheres and the complexity therein can be questioned. To address this we will discuss the relationship between single particle and bulk sample (or particle ensemble) non-spherical scattering phase functions through comparison with data from the Amsterdam-Granada Light Scattering Database.

Future work will be done towards expanding the system to include the collection of polarized light, with the ultimate goal of retrieving Muller matrix elements for a full description of scattering on the single particle basis. We also aim to expand the temperature regime of the EDB beyond that of Earth for atmospheric studies relevant to other solar system bodies and ‘cooler’ exoplanets.

5IM.2

Dual-Beam Optical Tweezers Development for Measuring the Dynamic Evolution of Aerosol Surface Tension and Viscosity. Aidan Rafferty, KYLE GORKOWSKI, Thomas Preston, *McGill University*

Understanding the evolution of glassy particles in the atmosphere has important implications when modeling mixtures of inorganic and organic particles. A glassy state of organic particles affects the particle to gas phase partitioning of organic species, diffusion of oxidants into the particle and the phase state of clouds, as they can serve as heterogeneous ice nucleating particles. To better understand how glassy states, evolve in the atmosphere as humidity and aerosol composition changes we have built a dual-beam optical tweezers (D-BOT).

The D-BOT system has two optical potential wells which trap a single droplet in-between them. The optical potential wells balance each other, pulling equally on opposite sides of the droplet. By increasing the laser power in the traps, the optical force pulling on opposite sides of the droplet causes it to deform into an ellipse. The surface tension of the droplet balances the optical force resulting in the elliptical deformation. We use the equilibrium deformation at high laser power to measure the surface tension of the droplet. Then after a viscous system has been deformed to an ellipse, the droplet viscosity is measured from the relaxation back to a sphere when the laser power is lowered. The physical dimensions of the ellipse and effective refractive index are retrieved from a newly developed fitting program for the measured elliptical whispering gallery modes (WGMs). The differences between the optical pathlengths for the major and minor axis of the ellipse result in shifts in the WGMs. These shifts in the WGMs are used to retrieve the ellipse deformation in the major and minor axis. We will present the new WGM analysis method for elliptical WGMs and with it, we will present results on surface tension and viscosity measurements for simple chemical systems.

5IM.3

Anatomy of Single Airborne Aerosol Particle Using Laser-trapped Submicron Position-resolved Temporal Raman Spectra. Aimable Kalume, Chuji Wang, Joshua Santarpia, YONG-LE PAN, *U.S. Army Research Laboratory, Adelphi, MD*

The study of various molecules located in different positions within a micro-sized particle in its natural phase is essential to a deeper understanding the functions of these molecules, such as the reaction of DNA, RNA, and protein molecules within a cell in buffer solution or different molecules within an airborne aerosol particle freely suspended in the atmosphere as they respond to various environments. Here, we present a new method that can measure the time-resolved Raman spectra from multiple sections across a laser-trapped single airborne particle to capture these crucial functions. Submicron resolved (up to 200 nm × 200 nm) temporal Raman spectra from different positions in a laser trapped particle can be obtained. Droplets in super micron size composed of diethyl phthalate (DEPh), glycerol, or their mixture have been used to test the new method. The results directly demonstrated the micro-cavity enhanced effects within a droplet, also the morphology, dynamics of phase-separation and evaporation of the mixed droplet. By inspecting the physical structure of the mixed droplet, we learned that the two liquids quickly separated and formed a core-shell-like morphology, in which the glycerol was mostly concentrated in the core, and the DEPh dominated around the outer layer of the droplet, as the mixed liquid was aerosolized. We also found that DEPh emerged to the surface and evaporated more quickly, then the glycerol evaporated slowly, but both chemicals in their mixed droplet evaporated much faster than that in their own pure droplet forms. This method should supply a powerful tool for monitoring various chemical reactions and understanding molecular functions at different locations within a single cell, spore, or particle in life and atmospheric science.

5IM.4

Design and Application of Aerosol Optical Tweezers to Explore Temperature Effects on Phase Separation and Acidity of Organic Aerosol at Subzero Temperatures. HALLIE BOYER, Kyle Gorkowski, Neil Donahue, Ryan Sullivan, *Carnegie Mellon University*

Phase and morphology in atmospheric aerosols are critical for understanding gas-particle and particle-cloud interactions, yet they remain hard to measure and predict due to multiple operative processes and properties. Further, there is currently a lack of data needed to train predictive models for explicit temperature dependence, especially data obtained from direct measurements on particles rather than bulk solutions. Phase separation is governed by ambient conditions and particle properties that are difficult to measure in situ, such as particle composition, interfacial tensions, and pH; thus, predictions frequently rely on a bulk perspective. Liquid-liquid phase separation can result in a core-shell or partially-engulfed morphology, where the aqueous phase is the core of the particle and the organic phase is present either as a complete shell or included lens, respectively. In the atmosphere, the morphology of the particle and the presence of an organic surficial layer can profoundly affect the particle's ability to scatter light and interact with chemical vapors and water. We directly determined pH, surface tension, and morphology of optically levitated particles using cavity enhanced Raman spectroscopy while monitoring changes in ambient conditions, including chemical composition and temperatures ranging from -20 to 40 C.

We use an aerosol optical tweezers (AOT) platform with a new chamber design for the integration and real-time measurement of particle properties under relative humidity and temperature control. Previously, we determined particle morphology of secondary organic aerosol in the AOT and identified core-shell and homogenous morphologies in response to organic vapor condensation and relative humidity. In the new chamber, we have explored the effects of pH and surface tension on phase mixing of multicomponent aerosol particles and investigated sub-zero temperatures of each property. The AOT provides steerable, contactless traps for single droplets of ~5 micron radii. Particles trapped in the AOT can reach metastable states, such as sub-cooled liquid states or supersaturation of solute with respect to solvent or other solute species, enabling measurements where data are scarce due to inaccessibility in bulk experiments. We determine surface tension by analysis of elastic backscattered light induced by the coalescence of two droplets trapped in a holographic optical trap. Surface tensions are necessary for predictions of particle morphology using spreading coefficient analysis, to predict aerosol interfacial composition, as well as for determination of cloud activation through Köhler theory. Finally, measurements of surface tensions as a function of temperature are applied to an analytic surface thermodynamic model to produce accurate predictions of interfacial tensions where little or no experimental data are available.

5IM.5

In-Situ Characterization of Aerosol Nanoparticles at Close-To-Ambient Conditions by Small Angle X-Ray Scattering (SAXS).

PAULUS S. BAUER, Heinz Amenitsch, Bernhard Baumgartner, Christian Rentenberger, Paul M. Winkler,
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The characterization of airborne particles is one of the main tasks in aerosol science. Especially the analysis of nanoparticles below 100nm requires particular attention, since they exhibit highly dynamic behavior that may impact cloud properties and hence global climate (IPCC, 2013). To determine the size and number concentration of aerosol nanoparticles Differential Mobility Particle Sizer (DMPS) and Condensation Particle Counter (CPC) are mostly used. A common drawback of these techniques is that they remove the aerosol particles from their original environment. Thereby, nanoparticles can get modified (e.g. by evaporation) or get lost (e.g. by wall collisions inside the instrument), which may affect the measured size distribution and concentration (Wang, J. et al. (2002). J. Aerosol Sci. 33, 6, 843).

An in-situ measurement technique can overcome these shortcomings of the conventional aerosol instruments. Small-angle X-ray scattering (SAXS), commonly used in material science or in biochemical process analysis, can fill this gap. It is capable of measuring in-situ particle size distribution in the nanometer range (Sztucki, M. et al. (2007), J. Appl. Phys. 101, 114304. Laksmono, H. et al. (2011), Phys. Chem. Chem. Phys. 13, 5855). These studies were operated with extremely high nanoparticle concentrations of ~10^{12}/cc and carrier gas pressures ~2 kPa to acquire proper SAXS signals. Conventional aerosol instrumentation on the other hand typically requires measurement conditions close to ambient pressure and concentrations not exceeding 10^{6}/cc.

Here we report synchrotron-based SAXS experiments on nanoparticle characterization. To provide a representative environment for aerosols a flow tube was operated at ambient pressure and concentrations of about 10^{6}/cc. This leads to a very low volume fraction of about 10^{-10} (see Beaucage, G. et al. (2004), Nat. Mater. 3, 370). A critical aspect for SAXS experiments with aerosols and this low volume fraction is the background scattering signal originating from the carrier gas. The air background usually is of the same order of magnitude as the signal from the nanoparticles. This issue was lately resolved by replacing air with helium as carrier gas. The usage of helium provides the opportunity of operating the flow tube under ambient conditions (temperature, pressure), and permits the parallel sampling by modified state-of-the-art aerosol instruments like CPC and DMPS system. To complete the picture, electron microscopy images were taken from aerosol samples.

5IM.6

Aerosol Spark Emission Spectrometer (ASES) for the Measurement of Trace Metals Concentration in Particulate Emissions from the Combustion of Coal in a Household Heating and Cooking Stove. NATHAN REED, Yixiang Zhang, Zhichao Li, Sameer Patel, Jiayu Li, Zehua Wang, Lina Zheng, Pramod Kulkarni, Pratim Biswas, *Washington University in St. Louis*

A recent study by the World Health Organization found that 92 % of the world's population lives in regions with unsafe ambient air quality. This situation challenges us to identify the source of pollutants, investigate their properties, and understand how they affect health and the environment. Investigating the properties of pollutants, especially particulate matter (PM), is critical for understanding both their source and subsequent effects. Based on its chemical composition and physical characteristics, PM can be attributed to sources such as coal powerplants, vehicle emissions, or biomass combustion. Although the mass concentrations of PM (PM1, PM2.5, and PM10) are almost exclusively used to regulate air quality, other physical metrics, such as number concentration, surface area, and even chemical composition might be a better way to represent the health effects of PM [1].

The accessibility and affordability of instruments critically hinder the comprehensive characterization of PM. Low-cost and compact instruments are being developed to measure the characteristics of PM in real time. These measurements currently are limited to the aerosol physical properties such as mass concentration and size distribution [2, 3]. Low-cost portable instruments to capture organic and inorganic species have not yet been developed thus these measurements are usually done by collecting filter samples for off-line analysis. Instruments that could perform chemical analysis in situ would reduce sampling costs, logistical problems, and measurement artifacts from storage and transportation of filter samples.

This work focuses on a portable instrument, the aerosol spark emission spectrometer (ASES) for quantitative characterization of the elemental content of PM. This instrument employs atomic emission spectroscopy using spark microplasma as the excitation source [4, 5]. PM is collected on the tip of a cathode in a coaxial electrode system via a one-step charge-and-collect scheme using corona discharge [6]. The collected sample is then ablated and excited by the spark microplasma, and the resulting atomic emission is recorded by a broadband CCD spectrometer for elemental identification and quantification. The utility of the ASES is demonstrated in this study by applying it to measure elements present in PM emitted from a solid-fuel cooking and heating stove. These stoves are one of the biggest contributors of PM emissions in countries such as India and China. In addition to real-time measurements from the ASES, filter samples were collected and analyzed using an ICP-MS to assess the accuracy of the real-time performance. In addition to measuring the elemental composition, we also used various real-time instruments to track the different phases of the burn-cycle in the stove, and to correlate physical PM metrics and elemental composition measurements.

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5IM.7

Measuring Functional Group Composition in Complex Environmental Samples: Infrared Photodissociation of Ions from Secondary Organic Aerosol. Emma Walhout, Jonathan Martens, Giel Berden, Jos Oomens, Jesse Kroll, RACHEL O'BRIEN, *College of William and Mary*

Secondary organic aerosols (SOA) are a large fraction of the organic particulate matter in the atmosphere with impacts on climate, air quality, and human health. The effect of aerosols on the climate is one of the largest uncertainties in estimates of radiative forcing. Much of this uncertainty is driven by the complexity of the organic fraction, with thousands of different molecules in an aerosol population. Mass spectrometry can be used to analyze the molecular composition of organic aerosols, however, information on the chemical structure and functional groups is typically lost with this type of analysis. By combining information on the functional groups and the molecular formulas in an aerosol sample, we can work towards identification of individual molecules in the mixtures. Infrared multi-photon dissociation (IRMPD) uses IR radiation to fragment ions in a mass spectrometer. With a tunable free electron laser as the light source, an action spectrum for ions can be generated in the fingerprint IR region (~600-1900 cm-1). These spectra, in combination with the fragment ions (MS/MS type fragments), provide details on the chemical structures of the ions. In this work we present the first application of IRMPD analysis, using the FELIX tunable free electron laser, to characterize compounds in SOA produced via ozonolysis of a-pinene.

5IM.8

Bounding Uncertainty in Functional Group Reconstruction of Organic Carbon and Organic Matter Concentrations in PM2.5 For the Improve Monitoring Network. MATTEO REGGENTE, Ann Dillner, Satoshi Takahama, *EPFL*

Functional group analysis by Fourier Transform Infrared (FT-IR) spectroscopy provides a chemically informative representation of the organic matter (OM) mass in aerosols. The molecular mixture conceptualized as a collection of functionalized carbon atoms can be used to estimate organic carbon (OC) content, degree of oxygenation, oxidation state, and organic matter to organic carbon mass (OM/OC) ratios for a large portion of the aerosol organic fraction (Takahama and Ruggeri, 2017). In previous work, this technique has been used to provide complementary information to mass spectrometry measurements which provide molecular speciation for a small fraction of the mass, or mass fragment composition commonly used for OM characterization (e.g., Faber 2017).

Functional group calibrations are typically prepared in the laboratory using simple mixtures and extrapolated to ambient aerosol spectra which contain a diverse set of compounds. While the potential of FTIR for quantitative aerosol research using this approach has been studied in separate contexts, a thorough investigation into the consistency of functional group estimation has not yet been conducted. In this work, we systematically explore the influence of spectral processing (e.g., baseline correction), selection of laboratory standards, and calibration algorithms on predictions of functional group distributions. Using 250 laboratory standards and 794 ambient sample spectra from 7 urban and rural sites in the IMPROVE monitoring network, we present the range of predictions that are possible under different assumptions. We also compare the physically-based peak-parameter representation for building calibration models to statistically-based multivariate regression models and their contrasting strengths, particularly for constraining the carbonyl apportionment to carboxyl and other non-acid functional groups. We also identify samples with higher loadings of larger particles from mineral dust and other sources that lead to excessive scattering and the Christiansen peak effect, which affect the quality of predictions. Directions for future research resulting from this analysis are presented.

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5MS.1

Spark Production of Internally Mixed Nanoparticles by Oscillating Sparks. Jicheng Feng, Nabil Ramlawi, George Biskos, ANDREAS SCHMIDT-OTT, *TU Delft*

We show that spark synthesis of mixed NPs allows a virtually unlimited number of combinations. Oscillating sparks are produced, in which cathode and anode are periodically exchanged with a frequency of around 10 MHz during a discharge time in the order of 1 µs. Nanoparticulate alloys of materials immiscible in the bulk can be produced this way. We show that the mean composition can be tuned through the spark characteristics and that a model predicts the broadness of the distribution.

5MS.2

Scaling-up of Extractor-Free Electrohydrodynamic Emitter Arrays in Linear Configuration. Nikolas Sochorakis, Jordi Grifoll, JOAN ROSELL-LLOMPART, *Universitat Rovira i Virgili*

Simultaneous operation of multiple electrospray emitters (multiplexing) have been used in virtually every known application of electrospray, to achieve relevant production rates: Pharmaceutical particle synthesis, surface coating, micro-electronics cooling, mass spectrometry in nanoelectrospray mode, microprotein arrays, 3D printing, microcombustion, and colloidal propulsion of spacecraft. Most often, electrospray emitters are arranged either in square or hexagonal 2D patterns, or in a straight line, as in the present study. When the concentration of the emitters is raised, the electrostatic interactions between the Taylor cones result in non-uniform electrical field, which can interfere with the spraying. Therefore, an important aim in this field is the development of configurations which allow robust, stable spraying.

Often, to achieve this goal, the electrospray emitters are positioned very near the counter electrode. In this way, the Taylor cones are shielded from one another and from the spray charges. When such counter electrode is a conducting ring or perforated plate, in order to extract the generated aerosol, this electrode is called 'extractor'. Since operating configurations with extractor electrodes can become challenging, at the beginning of this research we had reasoned that they would not be required in 1D arrays. Therefore, we have developed and evaluated extractor-free linear designs. In them, the counter electrode is much farther from the Taylor cones than the inter-cone spacing (or pitch) (about 4 times or more), and 'blind emitter' electrodes are placed at the ends of the array. At the same time, a backplate electrode is positioned behind the emitters, set at the same electrical potential.

We have characterized the conditions leading to stable cone-jet mode and spray plume behaviour as a function of the geometrical parameters of the arrays and the relevant liquid properties (e.g. electrical conductivity). We find that:

(1) It is possible to produce stable spraying along the entire linear array without the aid of extractor-type electrodes, over wide ranges of the applied voltage, using two blind emitter electrodes are located at either end of the array;

(2) The electrical potential difference needed to sustain stable spraying increases with the number of spraying emitters in the array, yet tends towards an asymptotic value, thus becoming finite regardless of array length;

(3) In long arrays, there are three distinct regions: an 'inner' central region, in which the sprays shapes are similar, unaffected by the length of the array; and two 'outer' regions, located at the ends of the array, where 'end effects' are concentrated, in which the sprays become broader.

(4) At high electric field strength, the spray symmetry breaks, as the Taylor cones retract towards the emitter tube (upstream) while they misalign, similarly as found for electrospying from single emitters, except in the linear array the direction of the emission is "seeded" by errors in the emitters' positions.

5MS.3

Magnetic Nanoparticle Chain Formation in a Combined Electric and Magnetic Field. CALLE PREGER, Knut Deppert, Maria E Messing, *Lund University*

Magnetic nanoparticles have been widely studied due to its many interesting properties and for their potential use as magnetic memory device and in medical diagnostic. Aerosol technologies provides a good mean to produce magnetic nanoparticles and the spark discharge generation of engineered nanoparticles enables formation of complex alloys with controlled size and concentration in a broad size range without agglomeration. The nanoparticles are typically deposited onto a substrate by using an electrostatic precipitator (ESP) and as the concentration of particles on the substrate increases random clusters are formed.

In this study, magnetic nanoparticles have been generated by spark discharge and the clusters formation on the substrate has been studied after the nanoparticles have been exposed to a magnetic field. We will show that it is possible to assemble individual nanoparticles into chains of magnetic nanoparticles in the presence of a magnetic field. The sparsely spaced nanoparticles are exposed to a magnetic field in the aerosol flow, the particles attract and collide and form chains of particles enabling formation of structures not possible with an electrostatic precipitator (ESP) alone. We will show the combined effect on magnetic nanoparticles from a magnetic field prior to deposition and from an electric field at deposition. This enables standing chains of nanoparticles and in some cases arcs of nanoparticles. By varying the strength of the magnetic field, the time the particles are exposed to the magnetic field, the concentration of particles in the gas flow and the size of the particles differently sized chains and shapes are formed and deposited on the substrate.

5MS.4

3D Nano-Printing via Electric-Field Assisted Aerosol Lithography. WOOIK JUNG, Yoon-ho Jung, Mansoo Choi, *Seoul National University*

Ion assisted aerosol lithography (IAAL) is an aerosol-based 3 dimensional (3D) assembly technique, which utilizes electrostatic focusing effects to manipulate the trajectory of incoming charged nanoparticles. (Kim et al., 2006; Lee et al., 2010; Choi et al., 2015.) Charged aerosols can be directed into openings in photoresist patterns or apertures in masks, making it possible to produce 3D nanoparticle structures whose shapes are defined by the cross-section of the openings in the photoresist layer or the mask.

Building upon this, here we show that translating the mask during the nanoparticle deposition process holds promises to be a novel 3D nano-printing technique. The shapes of the 3D nanoparticle structures are now determined not only by the cross-section of the mask openings, but also by the mask trajectory. Interestingly, we found that varying the horizontal mask translation speed leads to two distinct process regimes: ‘3D growth’ mode at slower translation speeds and ‘3D writing’ mode at faster translation speeds.

In ‘3D printing’ mode, high aspect ratio nanowires can be assembled by vertical upward translation of the mask during particle deposition. In principle, the process can continue indefinitely by matching the mask translation speed to the vertical growth rate of the structures. Adding horizontal components in the mask motion allows for creation of structures with various 3D shapes, such as slanted pillars or helices. In ‘3D writing’ mode, faster horizontal translation of the mask causes the particles to land next to the existing clusters rather than being deposited on them. This enables particle assembly whereby the structures do not lift off vertically from the substrate. Multiple sweeps of a given trajectory while depositing particles allow the clusters to grow in thickness and become ‘walls’.

In addition to the presented capability of directly printing 3D shapes using this technique, the ability to switch the aerosol material on demand with relative ease contributes to the expected versatility of this process, and further development and fine tuning will benefit applications that require multi-material 3D nanostructures.

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5MS.5

Low Temperature Plasma Synthesis of Pure and Uniform III-V Semiconductor Nanoparticles from Bulk Metals. NECIP BERKER UNER, Elijah Thimsen, *Washington University in St. Louis*

III-V semiconductors constitute a major component of optoelectronic materials. Although the synthesis of many of the III-V materials in nanoparticle form, for example GaAs, InP and InSb, has been well developed, stibnide and nitride particles still do not have an established general route of synthesis. The difficulties in the synthesis of these materials stem from the unavailability of chemically pure precursors or the extremely toxic nature of their chemical precursors, and the very high melting point of nitrides. In this work, aerosols generated from evaporation and condensation of pure bulk metals are utilized as precursors. These aerosols were mixed and then sent into a low temperature plasma (LTP) of argon. It has been recently shown that metal particles vaporize in the LTP despite the low gas temperature, and the generated vapor leads to the formation of monodisperse particles via a process involving nucleation and condensation [1]. Accordingly, the LTP was used to form the III-V compound nanoparticles by vaporization of the feed aerosols, followed by nucleation and condensation. Coagulation is largely prevented due to unipolar negative charging. The process yields nanoparticles which are monodispersed, spherical, crystalline and stoichiometric. This study focuses on the synthesis of Ga-based III-V semiconductor nanoparticles, and results on the synthesis of GaSb and GaN will be reported. Aerosols of pure Ga and pure Sb, and gaseous nitrogen bearing species were used as the precursors. Extensive ex-situ characterization of the produced materials by high resolution transmission electron microscopy, energy dispersive x-ray spectroscopy, electron-energy-loss spectroscopy, x-ray diffraction and inductively-coupled plasma optical emission spectroscopy will be presented. Operation of the aerosol sources will also be discussed.

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5MS.6

Easy On-demand Aerosol Doping Process to Fabricate Safer Antimicrobial Telluride Nanocomposites. DAE HOON PARK, Milan Gautam, Sung Jae Park, Jungho Hwang, Jong Oh Kim, Jeong Hoon Byeon, *Yonsei University, Korea*

On-demand synthesis of telluride nanostructure was developed from single-pass aerosol-based process under ambient gas flow conditions. Te nanoparticles(NPs) were assembled with Ag or Cu NPs using 4-Rod spark ablation system. Te NPs were partially alloyed with Ag or Cu NPs, resulting in 6 different formations of telluride nanocomposite. Then, their antimicrobial abilities were evaluated and compared with Ag, Cu and Te NPs. The minimal inhibitory concentration (MIC) values of the telluride nanocomposite against both Gram-positive bacteria (S.epidermidis) and Gram-negative bacteria (E.coli) were comparable to which of Ag or Cu NPs (that are famous as the antimicrobial agents) and their in vitro cytotoxicity was lower than which of Ag or Cu NPs as well. The simple on-demand doping process proposes a novel platform to constantly fabricate nanostructures which have safer antimicrobial activity without significant cytotoxic effects and environmentally friendly process.

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5MS.7

Plasma Synthesis of Mass-Produced CNT Materials. BRIAN GRAVES, Jean de La Verpilliere, Simon Engelke, Fiona Smail, Michael De Volder, Adam M Boies, *University of Cambridge*

The exceptional mechanical, thermal, and electrical performance of carbon nanotubes (CNTs) makes them ideal for a wide range of applications, however they are costly to produce and difficult to integrate effectively with other materials. We have developed a microwave plasma based process that can continuously synthesize several novel gas-phase CNT materials.

The presentation will demonstrate how transition metal catalyst particles are nucleated from the plasma and CNTs are grown from these particles in a furnace via gas-phase CVD. With this approach, a CNT-metal oxide hybrid material has been produced for use in lithium ion battery anodes. Findings from battery cycling demonstrate how this material offers increased storage capacity, greater cyclability, and a higher resistance to degradation from high discharge powers. Additionally, it is also possible to produce CNTs for structural and thermal applications. If the CNTs can achieve a sufficient length and number concentration they coagulate to form an aerogel which can be extracted continuously from the reactor. The self-assembled CNT structure can be wound to form fibres and mats which can be easily integrated into composites, wires, and heat pipes, among many other applications.

This plasma-based process exhibits several key advantages over other techniques. The extremely high temperature of the plasma permits vaporization of a wide range of precursor materials, including those in powdered, elemental form which are ideal for an industrial process since they are cheap and readily available. The plasma also has a high energy density, meaning that a large material throughput can be achieved with a small system. Large-scale production of these materials with this method could contribute to significant advances in materials for an array of engineering fields.

5MS.8

Nanographene Aerosol Production from Natural Gas by Microwave Plasma. RANDY VANDER WAL, Arupananda Sengupta, Evan Musselman, Kurt Zeller, George Skoptsov, *The Pennsylvania State University*

Graphene is the latest carbon allotrope, revolutionizing carbon science and igniting commercial interests. Synthesis processes are well known, beginning with mechanical exfoliation, varied graphene oxide (GO) routes and chemical vapor deposition (CVD). The former two processes begin with a pristine sp^2 carbon framework, with the GO path requiring its restoration. The CVD approach is by contrast a bottom-up approach in contrast to the former two being top-down approaches. It requires, however, a metal catalyst to activate the hydrocarbon decomposition and/or mediate the sp^2 framework formation. Without this metal an amorphous form of carbon forms, either as pyrolytic deposition if upon a surface or as a form of "soot" if as an aerosol. This presentation highlights aerosol (substrate-free) formation of graphene nanoplatelets in a microwave plasma. Whereas pyrolytic decomposition of hydrocarbons typically produces unstructured carbon, the nanoplatelets are characterized by dimensions of 200 – 500 nm, occurring in stack of 2-6 with morphology resembling mildly crumpled paper. Present selectivity is 50% +/- 20% on a solid carbon basis. Accompanying spectral diagnostics are used to characterize the reacting flow. Possible formation paths will be discussed. The co-production of hydrogen and high-value carbon materials from natural gas offers opportunities to reduce the costs associated with large-scale production of industrial or fuel hydrogen or platform chemicals while also producing synthetic, high-value carbon products such as the graphene nanoplatelets. H Quest Vanguard Inc. is developing microwave plasma processing of natural gas as a modular, compact and portable technology for production of hydrogen and premium carbon products.

5RA.1

Urban Substrates: Atmospheric Particle-bound Radionuclide Traps - The Example of Beryllium-7. PHILIPPE LAGUIONIE, Denis Maro, Luc Solier, Marianne Rozet, Didier Hébert, Pierre Roupsard, Olivier Connan, *IRSN*

In the context of chronic or accidental release of radioactive particles into the atmosphere, knowing atmospheric particle-bound radionuclide total (dry and wet) deposition flux on ground surfaces and the deposited radionuclide mobility is essential to assess risks both on populations and environment. Fluxes of deposition, of re-emission into the atmosphere, and of radionuclide transfer between rainwater and ground surfaces differ in urban and rural environments which are characterized by different surface types, heterogeneities and local micro-meteorologies. In particular, interactions between rainwater and urban surfaces have often been only considered as dry-weather deposited particles washing by rainwater flowing. First, this study investigated the ability of seven urban substrates (horizontal asphalt and grass, vertical façade coating and glass, and tilted zinc, slate and tiles) to permanently trap rainwater beryllium-7 at month scale. Beryllium-7 is a radioactive tracer naturally present in the environment (^{7}Be, $T_{1/2}$=50.3 days). Second, results were extended to a urban catchment (Pin Sec urban catchment in Nantes; area of 310 000 m²), knowing the repartition of each surface type in the total area of the catchment. The experimental set-up consists of two sets of each substrate: the first one was exposed to wet and dry atmospheric particle-bound ^{7}Be deposition whereas the second one was only exposed to dry deposition. The results showed that mean urban substrate retention rates present disparities linked to the surface orientation (main factor) and the substrate nature (secondary factor). Retention rates of horizontal, tilted and vertical surfaces were respectively between 65% and 93%, 48% and 59%, and 3% and 4%. The results also showed that the Pin Sec urban catchment area could trapped between 57 ± 25% and 83 ± 33% of the rainwater ^{7}Be at month scale.

5RA.3

Particle Emissions from Brakes – Sampling, Quantification and Characterization. MICHAEL ARNDT, Athanasios Mamakos, Klaus Augsburg, David Hesse, Fekix Wenzel, *AVL List GmbH*

With the exhaust of modern engines being cleaned up efficiently by aftertreatment systems, non-exhaust sources of particles (brake and tire wear) contribute significantly to the total amount of particulate matter emitted by today's vehicles. While tire wear emissions are difficult to quantify as they also depend strongly on the type of pavement, brake dust can be measured under laboratory conditions on a brake dyno. Researchers working on brake emissions employ a wide range of sampling and measuring techniques. The size spectrum of particles emitted by brakes is much broader than for combustion emissions. This results in specific requirements for the design of the sampling system.

In a dedicated measurement campaign on a specifically designed dilution tunnel installed in a brake dyno, different types of brake pads have been tested under various test cycles (WLTC, AK-Master) and specific baking manoeuvres simulating specific driving conditions.

It could be seen that moderate and more aggressive braking manoeuvres result in substantially different particle emissions (particle number, size distribution and PM mass).

Different instrument techniques have been used to quantify the particle emissions. Both thermally treated and untreated samples were sampled for particle number counting using CPCs with different cut-off sizes. Light absorption in the near infrared (i.e. by black carbon) has been quantified by using an AVL Micro Soot Sensor. Multiple PM filter samples have been collected by an AVL PM-PEMS to determine total PM emissions and to perform chemical analysis.

5RA.4

On-road Measurements of Secondary Aerosol and Size Dependent Number Emission Factors for Motorway Traffic Emissions across Europe Using a Mobile Laboratory Setup. MIIKKA DAL MASO, Joni Heikkilä, Miska Olin, Pauli Simonen, Antti Rostedt, Erkka Saukko, Heino Kuuluvainen, Joni Kalliokoski, Outi Potila, Anssi Järvinen, Mikko Poikkimäki, Topi Rönkkö, Jorma Keskinen, *Tampere University of Technology, Tampere, Finland*

Motorways make up a minor fraction of roads in Europe but carry a disproportionately large amount of traffic. Vehicle emission measurements have shown that highway driving at high engine loads may cause above average emissions of both primary and secondary particulate matter. These factors together make highways a significant source of air pollutants. Presently, comprehensive data of simultaneous primary and potential secondary aerosol mass measurements on motorways does not yet exist. We present data from three trans-European measurement expeditions that were carried out on highways reaching from Southern Finland to the Mediterranean, covering in total close to 8'000 km of highways. This dataset elucidates the relative fractions of primary and secondary emissions for highway driving, as well as gives new insights on the particle number emissions for highway driving.

The measurements were performed in 2015 and 2016 aboard the Tampere University of Technology Mobile measurement unit, a van modified to house a mobile laboratory setup, accommodating high-quality aerosol and trace gas observation setups. The modifications include a lithium battery powered inverter power supply with a supplementary charging generator powered by the van engine allowing continuous measurement instrument operation while driving. In addition, the van is fitted with aerosol and gas sampling lines, instrument installation shelving, a GPS and weatherstation, and a temperature regulation system. The sampling inlets were characterized with polydisperse aerosol and found to have good transmission efficiency for particles in the 1-1000 nm size range.

During the trans-European expeditions the instrumentation aboard the measurement unit consisted of aerosol size distribution instrumentation (Dekati ELPI), aerosol number concentration instrumentation (TSI and Airmodus CPC:s), trace gas detectors (CO_2, NO_x, O_3), and a fast-response oxidation flow tube (OFR) for the simulation the conversion of freshly emitted aerosol to photochemically aged aerosol (TUT Secondary Aerosol Reactor, TSAR). To bring the measured concentrations into the instrument's detection range, we used bridge dilution systems.

Measurements were predominantly performed on highways, with the driving speed over 80 km/h. The aerosol number concentrations were found to be clearly elevated in comparison to background. Motorway median number concentrations exceeded $4 \cdot 10^4$ cm^{-3}. On all expeditions, we found a significant fraction of particles in the sub-3nm particle size range, in line with recent findings that traffic is a significant source of nanocluster aerosol. Using CO2 data, we estimated average high-speed motorway driving number emission factors. Measurements using the the TSAR OFR showed that concentrations of potential secondary mass clearly exceeded the primary mass emissions, and our measurements also demonstrate that the high time resolution of the TSAR enables on-road emission factor determination of secondary aerosol.

5RA.5

Phenomenology and Sources of Submicron Aerosol Particles in a Mediterranean Harbour. BENJAMIN CHAZEAU, Grégory Gille, Boualem Mesbah, Brice Temime-Roussel, Henri Wortham, Nicolas Marchand, *Aix-Marseille Université, CNRS, LCE FRE 3416*

Marseille is the second largest city of France and the largest harbour of Mediterranean Sea. It is a challenging environment for air quality, combining an active photochemistry with high ozone concentrations and multiple anthropogenic sources including industrial activities (steel plant, refineries, and various petrochemical industries) and shipping (El Haddad et al. 2011). In order to document, on the long-term, the physico-chemical properties of fine particles, their sources and their evolution from day to multiyear period scales, we implemented an aerosol supersite in an urban background environment: Marseille-5avenues (MRS-5av).

In addition to air quality regulatory indicators (PM2.5, PM10, NOx, O3, SO2), we installed a ToF-ACSM (Time of Flight - Aerosol Chemical Speciation Monitor) for the analysis of the non-refractory fraction of submicron particles (OA, nitrate, amonium, sulfate) an Aethalometer (AE33) for the analysis of black and brown carbon (BC, BrC), an online metals analyser (Xact) and a SMPS (Scanning Mobility Particle Sizer) for the study of the aerosol size distribution (10-1100 nm).

A one-year real-time dataset collected between February 2017 and February 2018 is presented here. ToF-ACSM OA mass spectra were analyzed by means of Positive Matrix Factorization (PMF) using the multilinear engine (ME-2) approach (Canonaco et al. 2013). This dataset was also used to test a new time-dependent source profiles evaluation to capture the variability of the sources over the year. It was achieved by performing PMF on a rolling window and allowing the algorithm to best adapt to the current data. Such approach provides very valuable improvement for long time series dataset.

This analysis revealed very contrasted seasonal OA sources contributions and pointed out the overwhelming importance of local air masses circulation. Biomass Burning Organic Aerosol (BBOA), the dominant aerosol source during winter, is advected, mainly, from inland by nocturnal breezes. In such conditions, the total PM concentration can increase by up a factor of 5 in less than 15 min. During summer the OA mass concentration is dominated by secondary organic aerosol or more precisely oxygenated organic aerosols (OOA) but the most interesting feature regards the submicron particles number concentration and their size distribution. Very intense plumes (Ntot>100 000 cm-3) of ultrafine particles (Dp<80nm) associated with SO2 are observed systematically when sea breezes bring back over the city air masses impacted by industrial and shipping emissions.

5RA.6

PM2.5 and Its Chemical Composition in Sixteen Cities in Indonesia. MUHAYATUN SANTOSO, Diah Lestiani, Syukria Kurniawati, Endah Damastuti, Indah Kusmartini, Djoko Prakoso, Dyah Kumala Sari, Philip K. Hopke, Rita Mukhtar, et al., *Center for Applied Nuclear Science and Technology, BATAN*

The seasonal and spatial characteristics of PM2.5 and its chemical composition in Indonesia have been studied over a 3-year period (2014–2016) in sixteen big cities Indonesia covering Java, Sumatera, Kalimantan, Sulawesi, Maluku and Papua islands. Samples of airborne particulate matter were collected once a week for 24 hr using a Gent stacked filter unit sampler in two size fractions of 2.5 µm (PM2.5) and 2.5 to 10 µm (PM2.5-10). Black carbon (BC) was determined by reflectance and chemical elements analysis which performed by using Energy Dispersive X-ray Fluorescence (EDXRF). The measurement of chemical composition will be focused on the heavy metals concentrations for PM2.5. The annual mean of PM2.5 ranged from 4.13 to 20.5 µg/m3. The results showed that majority of the annual concentrations of PM2.5 in Java sites exceeded the annual average air quality standards (15 µg/m3), while for other sites are lower than the standards except Pekanbaru. During the period of forest fires in 2015, the daily concentrations of PM2.5 in Pekanbaru and Palangka Raya have exceeded the daily average national standard (65 µg/m3). While during the year 2016 the incidence of forest fires in both sites considerably reduced and the maximum concentration of PM2.5 are still below the standard. The PM10 annual mean concentrations for all sites were below national standards (150 µg/m3), while the average ratio of BC concentrations compared to the PM2.5 ranged from 10 to 27 %. Chemical composition of PM2.5 were also determined in order to understand the anthropogenic source of particulate matter. The results obtained in Surabaya and Tangerang sites showed that level of heavy metals in PM2.5 significantly higher than in other sites. These several findings significantly support the national programs of air quality improvement. The results can be used as an early warning, scientific research based references in designing and revising various government policies and regulations related air quality standards in Indonesia.

5RA.7

The Extinction Coefficient of the Aerosol over the Denver Metropolitan Area: Comparison with a Historic Data Set.

HELMUTH HORVATH, Paulus S. Bauer, *University of Vienna, Faculty of Physics, AEP*

Two identical series of optical measurements with the University of Vienna Telephotometer have been performed between July 23 and August 11 in the years of 1979 and 2017. Despite of being 38 years apart the same instrument and the same visibility targets have been used. During these 38 years the population of Colorado almost doubled from 2.8 to 5.6 Million, Boulder County's population increased from 130,000 to 300,000; Broomfield's population increased by a factor of more than 3, Denver City's population increased from 520,000 to 710,000, other surrounding communities also had a considerable population growth. Since human activities are also sources of particulate and gaseous emissions an increase in emissions has to be expected. On the other hand a series of new technologies has been introduced, e.g. exhaust gas cleaning of cars, thus a reduction in emissions per capita could be expected. Comparing the two datasets allows to see the result of the two counteracting effects.

The telephotometer was positioned on Gunbarrel Hill slightly north of Boulder and the spectral radiance of Mt. Morrison, slightly Southwest of Denver, was measured. Comparing the measured radiance with the radiance of the horizon behind the mountain, the extinction coefficient along the sight path can be determined. This sight path is between 100 and 800 m above the Greater Denver Area, and definitely also influenced by emissions in this area.

The weather conditions showed considerable variability, but this was the case in both years. Measurements performed during rain or fog (if possible at all) were excluded in the analysis reported below, so humidity growth of deliquescent particles needs not to be accounted for. Sometimes considerable haze screened the target, so optical measurements were not possible. In 1979 there was one day with considerable haze, so that no observations were possible. In 2017, there was also one day with considerable haze, but on about half of the days the extinction coefficient increased during the day and in the afternoon the target was obscured. This normally occurs when the mixing layer expands due to heating of the atmosphere by insolation.

The obscuration of the target makes a comparison difficult but still some conclusions can be drawn: Based on hourly measurements between 8:00 and 17:00, in 1979 the target was invisible 12 times during the measuring period. In 2017 it was obscured 29 times.

When being visible, the average measured extinction coefficient at 550 nm in 1979 was 46 Mm^{-1} with a standard deviation of 16 Mm^{-1}. For 2017 the corresponding values are 44 Mm^{-1} ± 18 Mm^{-1}, which can be considered the same value within the fluctuations. But this is only half of the story, since times where observations could not be performed were neglected. Therefore we included the data where no measurement could be performed as 100 Mm^{-1}, which is the minimum extinction coefficient needed to obscure the target. Obviously its value could be larger, the averages reported below are minimum values. Using these values, we obtain for the 1979 period an average of 51 Mm^{-1} with a standard deviation of 22 Mm^{-1} and for the 2017 period 60 Mm^{-1} ± 29 Mm-1. This can also be considered as indication of an increase in atmospheric extinction coefficient from 1979 to 2017.

The measured aerosol extinction coefficient was wavelength dependent, for about 85 % of the measured spectral extinction coefficients the Angström approximation (the extinction coefficient being proportional to λ^{α} with α the Angström exponent) could be applied. The Angström exponent is an indication for the mean size of the particles, the smaller α, the smaller the particles.

For the measuring period in 1979 an average α of -0.87 with a standard deviation of 0.36 was found, for the 2017 period the average was α=-1.24 ± 0.3. Therefore the particles in the air of 1979 were larger than in 2017. This is reasonable, since e.g. particles emitted by modern cars have become much smaller over the years.

5RA.8

Aerosol Chemical Composition Measurements from a Ship Campaign across the Mediterranean and Middle East during the Summer of 2017. JAMES BROOKS, Eoghan Darbyshire, Frank Drewnick, Stephan Borrmann, Hugh Coe, *University of Manchester*

The Middle East is home to over 200 million people, with the majority living in urban areas. The climate is hot and arid, with climate warming significant especially in summer months. It is well known that this region suffers from intense dust concentrations, as well as other aerosol species. The Mediterranean basin is an area encompassing a variety of environments and climates, with the region susceptible to both long-range transport of atmospheric aerosol from Europe, Africa and the Middle East, as well as local sources such as ship emissions. Although the Middle East and Mediterranean regions are a global change hot spot, they have received only little attention, e.g., in reports of the Intergovernmental Panel on Climate Change (IPCC, 2013). One reason is that observational data are insufficient, unavailable or of limited quality. In the past, studies needed to rely on satellite observations and sparse meteorological data. Atmospheric chemistry data are essentially non-existent.

There is a key relationship between aerosol and atmospheric chemistry. The reactive uptake of pollutant gases by mineral compounds can drastically change the particle properties, whereas the aerosols in turn influence the gas phase chemistry. Acidic pollutants can turn the particles from hydrophobic into hydrophylic, and convert them into efficient cloud condensation nuclei (CCN) (Karydis et al., 2011). This can alter the microstructure of clouds and increase removal of the particulates by deposition processes (Abdelkader et al., 2016). These processes have been found to be of key importance for Saharan dust that is transported over the Mediterranean basin and Middle East region.

The Air Quality and climate change in the Arabian Basin (AQABA) study aims to alleviate current scientific issues with unique field measurements, combined with satellite observations and high resolution atmospheric chemistry and climate modelling. A comprehensive ship-borne campaign took place from June-September 2017 measuring gases and particles in the Arabian Basin and the Mediterranean, studying the regional contrasts that occur in the atmospheric pollutants. The results presented here are collected from an aerosol instrument called a High-Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS), which collected aerosol chemical composition measurements. The presentation will summarise the key features in the regional aerosol burden for these regions, with an analysis into the sources of air masses.

Preliminary results show stark regional changes in aerosol chemical composition across the Middle East and the Mediterranean. Early highlights are very high sulphate and ammonia concentrations from a mix of local and long-transported sources in the Persian Gulf. Long range transported, highly oxidised organics in the Indian Ocean. Nucleation events in the Red Sea, coupled with high organics and sulphate concentrations throughout, especially in the Suez Canal region. And lastly, long range organics and nitrate concentrations in the Mediterranean, appearing to be sourced from mainland Europe.

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6AC.1

Aerosol Droplets Exhibit Stable pH Gradient. Haoran Wei, Qishen Huang, Linsey Marr, PETER VIKESLAND, *Virginia Tech*

Suspended aqueous aerosol droplets (<50 µm) are micro-reactors for many important atmospheric reactions. In droplets, and other aquatic environments, pH is arguably the key parameter dictating aqueous chemistry. The dynamic air/water interface of a droplet has the potential to significantly alter droplet pH from bulk water values. However, it is challenging to measure the pH inside single droplets due to their inaccessibility when using conventional pH meters. In this study, phosphate buffer droplets containing ≈75 nm gold nanoparticle (AuNP) based pH nanoprobes were collected onto a superhydrophobic substrate and scanned by laser confocal Raman microscopy. The Raman signal of the pH reporter, 4-mercaptobenzoic acid (4-MBA), was enhanced substantially through surface-enhanced Raman scattering (SERS) enabled by the AuNP clusters. By using these nanometer-sized pH probes the pH inside individual aerosol droplets was for the first time acquired. We show that the pH in a droplet is higher than that of bulk water by ≈3.3 pH units, which we attribute to the accumulation of protons at the air/water interface. The existence of this unexpected pH shift was corroborated by the observation that the catalytic reaction that only occur under basic conditions (i.e., dimercaptoazobenzene (DMAB) formation from 4-aminothiophenol (4-ATP)) occur within droplets, but not bulk solution. Results of three-dimensional scan also showed that the pH decreased from the droplet centroid to air/water interface. As the molar ratio of ammonia sulfate to phosphate buffer increased, the pH gradient decreased and finally was reversed indicating that the chemical compositions inside the droplet significantly affect its pH gradient.

6AC.2

Exploring Acidity in 1-10 µm Sized Liquid-Liquid Phase Separated Aerosol Particles. REBECCA CRAIG, Andrew Ault, *University of Michigan*

Secondary organic aerosol (SOA) formation and many of the subsequent multiphase chemical and physical processes SOA particles undergo are highly dependent on acidity. One such physical process is liquid-liquid phase separation (LLPS), which occurs commonly in atmospheric SOA particles. Relative humidity (RH), particle size, and chemical composition effects on LLPS have been characterized in laboratory studies, but few have focused on pH impacts on LLPS. Previous work has found that increasing pH corresponds to a decrease in the separation RH and that once LLPS occurs, the organic-rich phase is less acidic than the previously single phase particle. However, these studies have investigated primarily large particles (20-200 µm) at pH levels higher than what thermodynamic models predict for atmospheric aerosols. Herein, we investigate LLPS of laboratory-generated SOA particles composed of ammonium sulfate and polyethylene glycol 400 at atmospherically relevant sizes and pH's. Both bulk aerosol and individual particle pH are measured via established pH indicator paper and spectroscopic methods, respectively. The results of this study could have implications for acidity-dependent particle phase processes and how aerosol particle composition and morphology influence climate effects.

6AC.3

An Integrated Approach to Connecting the Chemical and Physical Properties of Aerosol. JAMES F. DAVIES, Michael Jacobs, Kevin Wilson, *University of California, Riverside*

Our ability to fully understand the effect of aerosols in the atmosphere requires a complete description of their physical and chemical state. Due to the highly oxidizing conditions in the atmosphere, aerosol particles are subject to heterogeneous oxidation, leading to their composition evolving over time. As composition evolves, so too do associated physical properties and characteristics, such as viscosity, hygroscopicity, surface tension, and diffusion. These factors regulate the ability of aerosols to act as sources of cloud condensation nuclei, influence their interactions with incoming solar radiation, and play an important role in the way aerosol affect air quality and human health.

Analytical techniques such as mass spectrometry and Raman/IR spectroscopy are powerful methods applied to measure the evolving chemical composition of aerosols and droplets. Single particle techniques, such as optical tweezers and electrodynamic balances, have been successful in measuring physical properties of aerosol particles, such as surface tension and hygroscopicity. The ability to combine these two types of measurement in a single experiment to resolve how physical properties change with an evolving sample composition could provide a fascinating new insight into how aerosol behave in the atmosphere.

Here, I report the coupling of a single particle levitator (a linear-quadrupole electrodynamic balance) to a high-resolution mass spectrometer.[1] Using electrospray-based ionization methods, the exact mass composition of single micron-sized droplets may be measured. Additionally, the physical properties of the droplets may be measured through the use of established methods, such as coalescence, isotope-exchange and humidity-cycling.[2] From these data, the physical characteristics of an aerosol can be directly linked to its chemical composition, providing a molecular-level insight into the factors that regulate the dynamics of aerosols in the atmosphere.

(1) Jacobs, M. I.; Davies, J. F.; Lee, L.; Davis, R. D.; Houle, F.; Wilson, K. R. *Anal. Chem.* **2017**, 89 (22), 12511–12519.
(2) Davies, J. F.; Wilson, K. R. *Anal. Chem.* **2016**, 88, 2361–2366.

6AC.4

Molecularly Resolved Atmospheric Aerosol Processes Studied in Single Levitated Particles Using Electrodynamic Balance Mass Spectrometry. ADAM BIRDSALL, John Hensley, Paige Kotowitz, Andrew Huisman, Frank Keutsch, *Harvard University*

A thorough representation of how atmospheric aerosol particle composition changes over their multiday lifetimes, and the consequent effects on climate and human health, requires a detailed fundamental understanding of the physicochemical system coupling the gas and condensed phases. For instance, individual compounds partition between the gas and condensed phase or can undergo particle-phase reactions.

Laboratory studies of aerosol particles have provided an opportunity to isolate systems of interest in a highly controlled environment and study them with specialized instrumentation. One approach in laboratory studies has been to analyze single levitated particles, largely with optical analytical techniques. We have extended the utility of this technique by coupling an electrodynamic balance, a method of suspending single charged particles (radius ~10 µm) in an electric field, to mass spectrometry. With this electrodynamic balance-mass spectrometry (EDB-MS) approach, we can understand with greater molecular specificity changes in particle composition under controlled laboratory conditions. Previous proof-of-concept work demonstrated the ability of our setup to quantitatively analyze the changing molecular composition of a model system.

Here we present the results of experiments that use EDB-MS to track the molecular evolution of individual aerosol particles, over timescales comparable to those of atmospheric particles. We have implemented instrumental modifications to improve our control of the environment surrounding the levitated particle, our particle sizing measurements, and our ionization source. With this refined setup, we have studied processes with atmospheric relevance.

First, we have measured the effect of interactions between organic and inorganic compounds on activity coefficients. The extent to which interactions between organic and inorganic compounds modulate particle-phase activities, and hence properties such as effective vapor pressures, remain poorly constrained. Activity coefficients can be extracted from EDB-MS data by fitting measured evaporation rates to a previously validated kinetic model of particle evaporation. Compared to levitated single particle experiments that track particle evaporation via change in particle radius, with EDB-MS we are able to use the mass spectra to monitor the evaporation of chemically speciated compounds within a multicomponent particle.

Second, we have studied nonradical, condensed-phase chemical transformations of organic compounds in single levitated particles. With EDB-MS, it is possible to identify with chemical detail the products of particle-phase chemistry as well as quantify the rates at which the chemistry takes place, as a function of parameters such as temperature and relative humidity. Compared to studies that take place in the bulk condensed phase, single-particle studies of chemical transformations represent a more realistic sample matrix in which the coupling of chemical and physical processes (e.g., partitioning between the gas and condensed phases) can be studied and highly concentrated conditions can be accessed.

The fundamental parameters extracted from these EDB-MS experiments (activity coefficients, chemical rates and equilibria) can be implemented in models to improve our representations of processes taking place in atmospheric aerosol particles.

6AC.5

Dynamics of Liquid-Liquid Phase-Separation Using Spatial-Resolved Raman Spectroscopy of a Laser-Trapped Mixed Organic-Organic Aerosol Droplet. AIMABLE KALUME, Chuji Wang, Joshua Santarpia, Patricio Piedra, Yong-Le Pan, *U.S. Army Research Laboratory*

Aerosols play key role in different areas including atmospheric processes, combustion, drug designing, household sprays, etc. Building upon our recent studies of characterizing a single-particle by laser-trapping Raman spectroscopy, a multicomponent organic-organic microdroplet from a mixture of diethyl phthalate (DEPh) and glycerol (1:1 initial volume ratio) suspended in air was investigated. Initial position-resolved examination of the droplet shows a gradient concentration at different positions within the droplet, suggesting phase separation. An extensive Raman spectroscopy measurement combining spatial and temporal resolutions, revealed the phase separation and the evaporation dynamics from the droplet. The DEPh–glycerol droplet presents a typical core-shell morphology, with a glycerol-rich core and DEPh highly concentrated within the outer layer. The reported approach provides a direct experimental observation of the morphological structure and the chemical microcomposition of a multicomponent microdroplet suspended in the ambient air. This technique opens new doors in probing surface enhanced phenomena, such as potential chemical reactions taking place at the interface of aerosols with the chemicals in the surrounding microenvironment.

6AC.6

Measurements and Modelling of Surfactant Coated Aerosol Particles. BRYAN R. BZDEK, Jussi Malila, Nonne Prisle, Jonathan P. Reid, *University of Bristol*

The surface tension of atmospheric particles is key to determining the critical supersaturation required for a particle to activate into a cloud condensation nucleus. Most models generally assume the surface tension of activating particles is equivalent to that of pure water. However, recent experiments have shown that the surface tension of particles can be much less than that of pure water, for instance due to the presence of condensed organic films, core-shell phase separations, and/or surfactants. Indeed, recent field studies have indicated that surfactants are important components of organic aerosol composition. For surfactants to be relevant to particle activation into cloud droplets, at least two parameters must be considered. First, the concentration of surfactant in the initial particle must be sufficiently large that surface tension depression is maintained over the course of activation, despite the dilution that occurs as water condenses onto the particle. Second, the high surface to volume ratio of micron and submicron particles necessitates partitioning of more surfactant molecules to the particle surface than in a typical solution, resulting in a depletion of the bulk concentration and an increase in the surface tension relative to a bulk sample.

This presentation will provide a comprehensive account of the size dependent partitioning behaviour of surfactant containing particles through a combination of measurements and modelling. The experimental approach utilises holographic optical tweezers, which allows quantification of the surface tension of picolitre volume surfactant-containing droplets. The measurement is accomplished by sub-microsecond resolved monitoring of the periodic shape oscillations resulting from controlled coalescence of two optically trapped droplets. Surface tensions are resolved to <1 mN/m. These experiments, when compared to bulk tensiometry measurements, demonstrate the surface-bulk partitioning effects in micron-sized droplets. Indeed, surface-bulk partitioning can result in a difference of >10 mN/m between the droplet measurement and the bulk measurement at the same nominal concentration. The experimental data are compared to a surface monolayer model that is constrained only by bulk surface tension measurements. This model agrees well with experimental observations, providing confidence in its treatment of particle surface-bulk partitioning. As a result, particle surface tension can be modelled to determine the sensitivity of particle surface tension to particle size and surface tension. This approach therefore will provide key information about the significance of the surface tension assumptions inherent in climate models.

6AC.7

Exploring Chemistry in Microdroplets in a Branched Quadrupole Trap. MICHAEL JACOBS, James F. Davies, Ryan Davis, Lance Lee, Frances Houle, Kevin Wilson, *Lawrence Berkeley National Laboratory*

Reactions in compartmentalized spaces are ubiquitous in nature, occurring in cells, mineral pores and aerosol droplets in the atmosphere. Recent studies have probed chemical reactions in a variety of different compartmentalized spaces, such as in an electrospray source, oil water emulsion, and thin films. These studies suggest that reactions in micron-sized compartments can occur at rates that are enhanced by several orders of magnitude compared to similar reactions in bulk solution. The experimental rate enhancements have been attributed to several different sources: increased concentration of reactants due to solvent evaporation, extreme pH in compartments due to large amounts of charge on the droplets, and interfacial effects due to the large surface to volume ratio of the compartments. While each of these explanations may play a role, a general explanation and the relative importance of each remains unclear. Ultimately, the source and generality of the observed rate enhancements has potentially far reaching implications for condensed phase aerosol chemistry as well as origin of life chemistry.

Here, I report work that has been performed using a recently developed single particle levitator (a branched quadrupole electrodynamic trap)[1] to study reactions occurring in micron-sized droplets. Using this trap, two 20-50 µm droplets with different compositions are contactlessly manipulated and merged to initiate a chemical reaction. Both the composition and size of the merged droplet are controlled precisely in the trap, and the evolving reactions within the droplets are probed spectroscopically (Raman) or with single particle mass spectrometry. From these measurements, the role of the air-water interface is isolated from concentration and pH effects, and its relative importance in enhancing reaction rates is determined.

(1) Jacobs, M. I.; Davies, J. F.; Lee, L.; Davis, R. D.; Houle, F. A.; Wilson, K. R. Anal. Chem. 2017, 89 (22), 12511–12519.

6AC.9

Validating a Surface Concentration Model. Anthony Toribio, Nonne Prisle, ANTHONY S. WEXLER, *University of California, Davis*

In 2013, Wexler and Dutcher published a paper using statistical mechanics to derive an expression for the surface tension of solutions over the full range of concentration from pure solvent to pure solute. The model only has a few free parameters yet was able to fit surface tension data for a wide range of organic and electrolytic solutes in water. In the current work we used the expression derived by Wexler and Dutcher along with the Gibbs adsorption isotherm for multicomponent systems to derive expressions for surface excess concentration. The parameters in the surface tension equation are the same as in the surface concentration equation, so if measurements are available for surface tension as a function of solute activity, the parameters can be identified and used to predict the surface concentration. In 2015 and 2016, Walz and coworkers published some of the first measurements of the surface concentration of alcohols on water; X-ray photoelectron spectroscopy was used to make the measurements.

In the current work, the derivation of the surface concentration equation is presented and the surface concentration predictions are compared with the measurements of Walz for 1-butanol, 1-hexanol, 1-pentanol, 1-heptanol, and t-butanol. The comparison sheds light on the model and measurements, but also on the meaning of surface excess concentration.

6AE.1

Characterization of Air Pollutants in Delhi during 2017. HAO GUO, Shovan Sahu, Sri Kota, Hongliang Zhang, *Louisiana State University*

Delhi is facing severe air pollution and the government has set up air pollutant monitoring network to inform the public and increase the understanding of air pollution events. One year-long air pollutants data collected from the network were analyzed in this study. This is the first time to the spatial and temporal variations of particulate matter with aerodynamic diameter less than 2.5 µm (PM2.5) and less than 10 µm (PM10) as well as gaseous species were studied in Delhi using hourly data from 8 sites during 2017. Delhi is facing tremendous air pollution as all major pollutants have concentrations reaching severe pollution levels. Seasonal variations are analyzed and correlations between different pollutants and same pollutants at different sites are investigated. In addition, three extreme PM2.5 events (hourly average concentration exceeding 300 µg/m3 for ~40 hours) are examined with the consideration of meteorological conditions. This study can greatly support the research on formation, transport and human health effects of air pollutants in Delhi and India.

6AE.2

Particulate Matter Concentrations from Urban Settings of Pakistan, China and Europe (UK). IRFAN ZAINAB, Zulfiqar Ali, Zona Zaidi, Syed Turab Raza, Zaheer Ahmad Nasir, Ian Colbeck, Liu Weilong, *University of the Punjab, Lahore, 54590, Pakistan*

Continental blanket of particulates over cities is disturbing sun energy trapping and grosses to atmosphere. Particulate matter (PM) is also the key component of air pollution that is directly thrown into the air by various natural and anthropogenic sources. Exposure to particulate air pollution has directly been associated to higher morbidity and mortality. Studies show that particulate matter is one of the six criterion pollutants and the most dangerous one accounts for 3.7 million premature deaths annually and nearly 88 percent of these deaths occurs in developing countries. Current investigations reveals indoor and ambient PM levels monitoring in urban settings of the major cities from UK, Pakistan and China. Student accommodations, public transports, and ambient residential settings were selected as study areas. Particulate matter emissions were monitored for twenty-four hours at each site except transport indoors monitoring that was for six hours. Latest DustTrak DRX (Model 8533, TSI Inc.) recently calibrated was used that simultaneously give the values of all fractions like PM_1, $PM_{2.5}$, PM_4 Respirable, PM_{10} and PM_{Total}. The findings conclude that the respective average values for PM_{Total} concentrations for Student accommodations in UK (61 μg/m³) was much lower than the rest of monitored countries with overall average, Pakistan concentrations (372μg/m³) was remarkably higher, while China was also found to be significantly polluted with 223μg/m³ of Particulate matter. On the other hand, Public transports were also monitored that showed remarkably higher level of PM concentrations with average PM_{Total} concentrations of 87 μg/m³ in UK, (372 μg/m³) in Pakistan and 151 μg/m³ in China. These persistent elevated PM concentrations shows the Ambient PM concentration levels have influenced indoor buses and transport facility that is serious health concerns for passengers. The ambient environment of UK, Pakistan and China results were supporting evidence with monitored respective values of PM total were 45 μg/m³ in UK, 121 μg/m³ in Pakistan and 110 μg/m³ in China. Weather and climatic conditions are not similar in these countries that certainly have influenced the fluctuations in the PM concentrations despite of other factors. Therefore, the origin and source of PM is alarming with significantly high figures than the air quality standards suggested by the WHO limits.

6AE.3

Secondhand Smoke Exposure during the Travel between United States and China: The Association with Urinary Biomarkers of Polycyclic Aromatic Hydrocarbons and Lipid Peroxidation. Yan Lin, Xinghua Qiu, YIFANG ZHU, *University of California Los Angeles*

Secondhand smoke (SHS) was among top risk factors to general population. Exposure to SHS might vary among countries due to different smoking prevalence and control policies, but it is unclear whether cross-border traveling would bring significant health risk from SHS exposure to international travelers. In this study, we followed 27 non-smokers traveling between Los Angeles and Beijing. Their urine samples (n=196) were collected before (LA1), during (BJ), and after (LA2) the trip for the measurement of biomarkers of SHS (i.e. cotinine), polycyclic aromatic hydrocarbons (PAHs) and lipid peroxidation (i.e. malondialdehyde and 8-isoprostane). The geometric mean concentration of urinary cotinine was 0.13, 1.50, and 0.22 µg/g creatinine in LA1, BJ and LA2, respectively. Likewise, hydroxylated-PAHs (OH-PAHs) were also significantly higher in BJ than LA1 or LA2 ($p<0.05$). The increase of urinary OH-PAHs in BJ was partially attributed to SHS exposure given its significant association with urinary cotinine ($p<0.05$). Urinary cotinine was positively associated with malondialdehyde and 8-isoprostane ($p<0.05$). These results indicated an increase of SHS exposure caused by the travel from Los Angeles to Beijing, which might further contribute to an increase in PAHs exposure and lipid peroxidation.

6AE.4

Vertical Variations in Outdoor Particulate Matter along the Height of a Tall Building in an Urban Environment.

PARHAM AZIMI, Haoran Zhao, Torkan Fazli, Dan Zhao, Afshin Faramarzi, Luke Leung, Brent Stephens, *Illinois Institute of Technology*

It is generally assumed that building height can affect indoor exposures to pollutants of outdoor origin in tall buildings, as some ground-level pollutants such as particulate matter may be diluted at higher elevations. However, we are aware of very few measurements of airborne particle concentrations that have been made along the height of tall buildings. Therefore, we conducted a pilot study to measure the vertical variation of environmental conditions, outdoor particulate matter, and several other outdoor pollutants along the height of a ~60-story (~300 m) building in downtown Chicago, IL during a one-week period in the summer of 2017. Simultaneous measurements of size-resolved particulate matter (0.3 to 10 µm, which were used to estimate PM1, PM2.5, and PM10 mass concentrations), were made using multiple sets of instrumentation installed in the outdoor air intakes of the mechanical systems on the 2nd, 16th, 29th, and 44th floors and in an open-air area on the 61st floor. The results demonstrate that PM1, PM2.5, and PM10 concentrations generally decreased approximately linearly with building height. The vast majority of measured differences were statistically significant. Most strikingly, the average PM1 and PM2.5 concentrations on the top two floors were more than 30% lower than on the 2nd floor. Moreover, we used a simple well-mixed mass balance model to demonstrate how the measured differences in particle concentrations along the height of the test building would likely manifest in differences in indoor concentrations of particles of outdoor origin in a typical office space.

6AE.5

Assessment of Personal Exposure to Particulate Emissions in Urban Microenvironments. Jie Rui Ngoh, Thi Minh Phuong Tran, RAJASEKHAR BALASUBRAMANIAN, *National University of Singapore*

Fine particles suspended in air (PM2.5) pose a threat to public health due to their ability to penetrate deep into the respiratory tract and migrate into the bloodstream. As a result, finding the sources of these particles and controlling their emissions are a top priority in many countries. Fixed air quality monitoring stations, equipped with expensive and bulky instruments, are widely used to measure PM2.5. However, these instruments have limitations because of their fixed positions and do not provide spatially representative PM2.5 readings. Furthermore, the PM2.5 concentrations provided by a single monitoring site may not accurately represent the particle concentrations around people distributed in its vicinity, who may be concerned about the health effects of PM exposure. Mobile and cost-effective PM2.5 sensors been developed in recent years to overcome this problem and to provide realistic data for human exposure assessment and urban air quality improvement.

We carried out a pilot study to assess personal exposure to mass concentration of PM2.5, sub-micron particle number concentration, Np, and equivalent Black Carbon, eBC, in diverse outdoor and indoor microenvironments (MEs) in Singapore, a densely populated country. A GPS receiver was used to track movement and exposure of individuals across the MEs. The novelty of this approach is that exposure measurements were taken across the full heterogeneity of places visited and activities conducted to gain as much insight as possible into an individual's total exposure. This is important as individuals are constantly on the move and follow their own activity patterns, which determine their individual exposure. Exposure to PM2.5, Np, and eBC varied considerably across the MEs because of changes in the particulate emissions from local sources in the immediate vicinity of MEs. Personal exposures to PM2.5 based on the data obtained from portable sensors were much higher those from fixed air quality monitoring stations. Mobile sensing could thus provide local environmental protection agencies with a comprehensive map of PM concentrations, at specific locations and at specific times, which allows for formulation of effective strategies to reduce PM emissions at the city scale.

6AE.6

Neighborhood-scale Spatial Variability of PM Mass and Number and Exposure Misclassification in an Eastern US City.

Hugh Li, Peishi Gu, Qing Ye, Naomi Zimmerman, Ellis Shipley Robinson, R. Subramanian, Joshua Apte, Allen Robinson, ALBERT A. PRESTO, *Carnegie Mellon University*

Long and short-term exposure to airborne pollutants are associated with adverse health effects. Regulatory monitors can be used to determine if their surrounding regions meet regulatory standards of air pollution. Measurements at monitors describe surrounding residents' air pollution exposure, help derive exposure dose response functions in epidemiology studies, and are essential input for chemical transport model and remote sensing. But evaluation is needed to assess spatial representativeness of monitors in different environments. We measured CO (traffic source marker), NO_2, ultrafine particle concentration (UFP), and PM_1 with a mobile laboratory in a post-industrial U.S. Eastern city (Pittsburgh, PA) in 2016. We sampled in ~1 km^2 areas in 15 neighborhoods representing different land use and exposure regimes (e.g., urban and rural, high and low traffic). Mobile sampling was conducted on up to 15 distinct days in each neighborhood to study fine-scale spatial variation in pollutant concentrations. Each 1 km^2 neighborhood was subdivided into 50 m cells for spatial analysis. CO and NO_2 exhibited within-neighborhood (~1 km^2) spatial variation, with hotspots elevated by up to a factor of 5 above the regional background. UFP was the most variable, with spatial variations up to an order of magnitude higher than background. PM_1 showed the least spatial variability. Spatial variability is driven by local sources, such as traffic at urban sites.

Mobile measurements convolve spatial and temporal variations in concentration, and we use multiple methods to separate these sources of variability. First, we compare observed spatial variations within each 1 km^2 neighborhood to typical hour-to-hour variations measured with a stationary monitor placed in the neighborhood. Spatial differences outside the interquartile range of hourly temporal differences are deemed significant. This analysis indicates that using a single monitor to represent the surrounding ~1 km^2 areas could introduce an average daily exposure misclassification of 46 ppb (S.D. = 26) for CO (30% of regional background), 3 ppb (S.D. = 2) for NO_2 (43% of background), 4000 #/cm^3 (S.D. = 1900) for UFP (64% of background), and 1.2 μg/m^3 (S.D. = 1) for PM_1 (13% of background). Exposure differences showed fair correlation (R^2 = 0.5) with traditional land use covariates such as traffic volume and restaurant density. Secondly, we used Wilcoxon signed-rank test to determine which 50 m cells represent the same underlying distribution of concentrations, and which are different. This test allows us to examine the robustness of our exposure misclassification calculations, and to determine the number of monitors required in each neighborhood to reduce pollutant exposure misclassification within 10%.

6AE.7

Early Lessons from New Air Pollution Exposure Science: High-resolution Mapping of Urban Air Quality using Google Street View Cars, Low-cost Samplers, and Aerosol Mass Spectrometry. JOSHUA APTE, Kyle Messier, Sarah Chambliss, Michael Brauer, Julien Caubel, Shahzad Gani, Steven Hamburg, Thomas W. Kirchstetter, Julian Marshall, Brian LaFranchi, Melissa M. Lunden, Chelsea V. Preble, Albert A. Presto, Christopher Portier, Allen Robinson, Ellis Shipley Robinson, Rishabh Shah, Karin Tuxen-Bettman, Roel Vermeulen, Ramon Alvarez, *University of Texas at Austin*

Human exposures to air pollution can vary sharply in space and time. Recent advances in measurement technology enable a rich understanding of the spatiotemporal patterns of outdoor air pollution that influence population exposures and environmental inequities. For example, carefully designed mobile sampling campaigns are now able to reveal patterns of long-term ambient air pollution concentrations at very fine scales (<< 100 m).

Here, we present an overview of the most extensive mobile air pollution measurement campaign conducted to date in a single urban area. Using two specially equipped Google Street View cars, we mapped spatial patterns of air quality in the San Francisco Bay Area between May 2015 and December 2017. The cars were outfitted with reference-grade instruments to measure NO, NO_2, black carbon (BC) and ultrafine particle number count at high time resolution (~ 1 Hz). During a 30-month campaign, measurements took place on most weekdays during daytime hours, resulting in a large dataset: ~10 million samples collected during > 4000 h, encompassing 100,000 km of driving. Additional sampling incorporated a dense network of low-cost samplers and a mobile aerosol mass spectrometer, as described below. The overall campaign consisted of several targeted investigations.

During an initial year of already-published measurements, we sampled every road 20-50× within three neighborhoods (~30 km^2) in Oakland, CA. Next, during 1.5 years of follow-up measurements, we mapped pollutant concentrations in rural, suburban, and dense urban neighborhoods throughout the SF Bay Area. These measurements reveal how the within-neighborhood pollution structure is overlaid on top of regional spatial gradients in air quality. Repeated measurements over the full 2.5-year period demonstrate persistent spatial variability over time. Patterns of NO, NO_2 and BC in Oakland had high correlation (r^2>0.85) between the first and second years of measurements. Shorter-term measurement periods (~1-2 months) were generally sufficient to reproduce overall spatial patterns, albeit with ±30% bias in mean concentrations relative to annual-average conditions.

We conducted an especially intensive multi-method study of the mixed residential/industrial West Oakland neighborhood during Summer 2017. Street View cars drove every street in this 5 km^2 domain during days, nights, and weekends to characterize the temporal evolution of spatial patterns in air quality. In parallel, a dense network of 100 BC monitors was deployed at fixed sites to characterize temporal patterns at fine spatial scales. Finally, a van with a high-resolution aerosol mass spectrometer (HR-ToF-AMS) repeatedly sampled all city streets in the same domain to collect data on non-refractory PM_1 chemical composition. We used positive matrix factorization of AMS data to identify source signatures that contribute to spatial patterns of air quality. Fixed and mobile measurements indicated that BC, NO, and other primary species were elevated on weekdays relative to weekends, with distinct shifts evident in spatial patterns within neighborhoods. UFP concentrations were less spatially variable, and exhibited a pronounced mid-day peak with only small weekday-weekend differences. Mobile AMS data demonstrate a temporal evolution of source and background contributions over the course of each day and spatial hotspots with elevated markers of primary emissions.

This campaign overview presentation (i) summarizes how routine mobile air pollution monitoring can reveal new information about spatial variability in population exposure to air quality, (ii) explores the methodological advantages and tradeoffs of alternative sampling approaches, and (iii) illustrates how established measurement techniques from the atmospheric sciences can add powerful new insights to studies of human exposures in urban areas.

6AE.8

Child Exposure to Indoor and Outdoor PM at Schools and Homes in the Lisbon Metropolitan Area, Portugal. VÂNIA MARTINS, Susana Marta Almeida, Tiago Faria, Inês Cunha-Lopes, Carolina Correia, Nuno Canha, Evangelia Diapouli, Manos Manousakas, Konstantinos Eleftheriadis, *C2TN, IST, Universidade de Lisboa, Portugal*

Numerous personal exposure studies have revealed poor correlations between outdoor ambient PM concentrations and personal exposure measurements. In fact, the personal exposure includes not only contributions from ambient PM sources, but also contributions from indoor, commuting and leisure activities, which depend on the lifestyle of each individual and the different microenvironments frequented, such as home, workplace, commuting type, etc. Since people spend most of their time (80 – 90%) indoors, it is widely recognized that a significant portion of total personal exposure to ambient PM occurs in indoor environments. Whilst the health effects of adult exposure cannot be neglected, children are more susceptible than young adults to air pollutants; therefore, their exposure is a major health concern.

This study aims to assess the indoor and outdoor PM concentrations at several schools and homes in the Lisbon metropolitan area (Portugal) to calculate the children exposure. In the scope of the European Project LIFE Index-Air, PM2.5 and PM2.5-10 samples were collected in parallel in the indoor and outdoor of 40 homes and 5 schools. Sampling was carried out during the occupied time: 8h at schools and 15h at homes. Once the gravimetric determination of the PM mass concentrations was performed, the chemical characterization of the PM collected on the filters was carried out. The elemental analysis of PM samples was performed with a high-resolution energy dispersive X-Ray fluorescence spectrometer; the elemental carbon and organic carbon fractions of PM was analyzed by a thermal–optical method, and Polyaromatic Hydrocarbons were analyzed by gas chromatography–mass spectrometry. After the chemical composition of PM the exposure of children to PM components was assessed.

In the absence of indoor air legislation for PM, the values found in this study can only be compared with limit values for ambient air. As indoor air quality is an important determinant of human health and comfort it is essential to establish regulations for indoor microenvironments. Generally, the PM2.5 and PM10 concentrations obtained in the outdoor spaces of the homes and schools were below the WHO guidelines.

LIFE Index-Air project (www.lifeindexair.net) is developing an innovative, versatile and modular policy tool that establishes a relation between children exposure to PM compounds, health effects and emission sources. This tool combines a pack of models to select cost-effective improvement measures to protect human health. The exposure module of the tool calculates exposure from outdoor PM levels, indoor-to-outdoor concentrations and time activity patterns.

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6AE.9

Descriptive Characterization of Personal Exposure to Fine and Ultrafine Particle Among Inner-City Children with Asthma. Ehsan Majd, KIRSTEN KOEHLER, Meredith McCormack, Nadia Hansel, *Johns Hopkins School of Public Health*

Introduction: It is yet to be determined which property (size, chemical composition, morphology) of particulate matter (PM) air pollution contributes most to its adverse respiratory effects. However, recent toxicological findings point to the potentially greater role of the smaller fraction of PM, known as ultrafine particles (UFP, particles with diameter less than ~0.1 µm). Recent advances in sensor technologies has facilitated the assessment of personal exposure to UFP at high spatial and temporal resolutions; an important step towards a better characterization of PM exposure and informing effective practices and policies to mitigate its harmful effects.

Methods: In this work we characterized personal $PM_{2.5}$ (particles with diameter less than 2.5 µm) and UFP exposures of 25 children aged 8-17 with asthma for 4 consecutive days at high spatial and temporal resolutions, aiming to answer two questions: 1) is personal exposure monitoring necessary for UFP in addition to $PM_{2.5}$? 2) is it necessary to monitor personal exposures at high temporal resolution? Personal $PM_{2.5}$ and UFP (expressed as LDSA, lung-deposited surface area) monitors were placed inside a backpack, which also contained a GPS and a data logger for collecting real-time information on geographic location, temperature, relative humidity, acceleration and light intensity at 10-sec intervals. Information about means of transportation used, places visited, and activities at home that may have resulted in high exposures were also obtained. We partitioned the measured personal exposures into five microenvironments (ME): home, school, vehicle commute, walk, and other (for the visited places other than home and school) and examined the distribution of exposures in each of them for different averaging times. We also calculated and examined the correlation coefficients between $PM_{2.5}$ and UFP exposures across the MEs.

Results: Among the MEs, both $PM_{2.5}$ and UFP exposures were dominated by home. Unlike $PM_{2.5}$, time-weighted averages of UFP exposure were high for vehicle commute (35±31 $\mu m^2/cm^3$) and walk (20±11 $\mu m^2/cm^3$) relative to home (37±23 $\mu m^2/cm^3$), despite very small fractions of time spent in these MEs (averages of 1% and 2%, respectively compared to 73% for home). Mean exposures did not vary much by changing the averaging times, but we observed drastic decreases in maximum $PM_{2.5}$ and UFP exposures by increasing the averaging time from 1 to 5 min for vehicle commute and other. Correlation between UFP and $PM_{2.5}$ exposures were generally high at home (R=0.72) and poor in other MEs. However, we observed several cases of weak correlations for home (high UFP and low $PM_{2.5}$), which occurred during the evening hours and coincided with common household activities, such as cooking and cleaning (sweeping, vacuuming, and using chemical cleaners).

Conclusions: Our findings suggest the importance of personal exposure monitoring at high temporal resolution and accounting for short peaks in urban environments. Moreover, we observed that personal UFP exposure was much more sensitive than $PM_{2.5}$ to activities inside an ME, as well as moving from one ME to another. Therefore, and considering its potentially greater health risks, we believe it is crucial to include UFP as one of the major variables of interest to personal exposure monitoring campaigns, especially for more susceptible population such as children with asthma.

6AM.1

A Computational Study of Electrostatic Focusing of Aerosol Nanoparticles Using A 3-Electrode Einzel Lens. RAYHAN AHMED, Ranganathan Gopalakrishnan, *The University of Memphis*

The focusing and deflection of electrons and ions using electric fields has been successfully harnessed for many applications and instrumentation development. An adjustable electric field can manipulate the flight path of an electron, ion or a charged particle. This study explores the possibility of focusing charged aerosol nanoparticles, which are much heavier compared to electrons and ions. The study revealed that charged nanoparticles could also be focused towards a focal point by applying an adjustable electrostatic field along the flight path of the same. This study introduces a non-dimensional parameter χ_e ($ne\Delta V/mU^2$), the ratio of electrostatic potential energy to the kinetic energy of an aerosol nanoparticle that greatly affects focusing performance. In the absence of collisions with gas molecules (vacuum), the sum of kinetic and potential energy of a particle remains almost constant, and the applied electrostatic field controls the direction of motion. In this study, the focusing device is a 3-electrode electrostatic lens where the electrostatic field deflects particle trajectories towards the central axis of the lens. The average focal length of the lens is seen to have an inverse power relationship with χ_e (i.e.) when χ_e is almost zero the focal length is infinity and decreases with the increasing χ_e. Multiple focal points appear when electrostatic potential energy is much larger than kinetic energy ($\chi_e > 3$ in this study). The focusing performance also depends on the electrostatic lens geometry and the attributes of the inlet particles - initial kinetic energy, direction of motion and particle beam radius at the entrance of the electrostatic lens. Similar to electron and ion optics, the focusing performance is limited by spherical aberration and beam divergence. Both χ_e and initial beam width seems to maintain a cubic relationship with spherical aberration, and the divergence angle has a quadratic relationship with χ_e which ultimately increases the spherical aberration. From this study, it can be inferred that better focusing performance i.e. a tighter beam of nanoparticles with minimum spherical aberration and small divergence angle could be achievable while $\chi_e<1$, initial particle motion is parallel to the central axis, and initial beam width is much smaller compared to the diameter of the focusing device. The generation of highly focused beam of nanoparticles is motivated by nano-pattern fabrication research that has numerous applications in electronic and plasmonic devices.

6AM.2

A Binary Nucleation Model for Engineering Layered Drug Nanoparticles from Air Jet Atomization of Two-Solute Solutions.

Y.S. MAYYA, Chandra Venkataraman, *Indian Institute of Technology Bombay*

It is well-known that the use of nanoparticles for drug delivery offers several advantages in terms of targeting the delivery and enhancing bioavailability, half-life and stability in biological systems. Encapsulation of drugs in lipids often enables multidrug (hydrophobic and hydrophilic) therapy and controlled release. Aerosol synthesis of layered, lipid-encapsulated drug nanoparticles, with surface stabilizing molecules, has recently been carried out through spontaneous self-assembly in evaporating sub-micron droplet aerosols generated through air-jet atomization of two-solute solution precursors. Air-jet atomization offers higher throughput rates of nanoparticles, over that from traditional electrospray systems, with coaxial geometries, used for layered nanoparticle preparation. A major question that needs to be addressed is whether it is possible to engineer encapsulation, in a selected lipid-drug system and control layer thickness and composition. In a recent theoretical paper, (Sapra et al. 2017) an attempt was made to answer this question by introducing a novel concept of "lipid-drug demarcation diagrams". The theoretical approach employed above consists of an evaporating droplet-solute diffusion model combined with a prescription of critical supersaturation solubility (CSS) for crust formation. Critical supersaturation solubility is determined from the criterion proposed by He et al. (2006), invoked from classical nucleation theory. A parameter space was defined of material properties and process conditions for the formation of a layered structure with the preferential accumulation of the lipid in the outer layer. The developed diagrams can guide the selection of solvents, lipids, and processing conditions such that drug loading and lipid encapsulation are optimized in large scale production of layered nanoparticles. However, the CSS concept is applicable strictly for single solute system. For nucleation in a two-solute system, the attainment of crust for one species will be influenced by the activity of the other. To take this aspect into account, it is then necessary to address the problem from binary nucleation framework. In this work, we develop a theory that combines binary nucleation process (Seinfeld and Pandis, 2006) inside the droplet, with the evaporating droplet-solute diffusion model model. It involves the formation of a compound two-species critical nucleus that rapidly grows into a crust by surface growth mechanisms. The composition of the outer layer is now quantified in terms of relative enrichment of lipid over the drug. The model predicts the kinetic growth of this layer until the porosity decreases to a level when the evaporation rate slows down considerably, when the model terminates to calculate nanoparticle diameter and shell thickness. Although complex, the model not only predicts the crustal diameter, but also delineates the propagation of solidification inside the particle along with the evolution of composition. Details will be presented substantiating improvement of this approach over existing solute diffusion models.

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6AM.3

Numerical Model for the Aerosol Formation Process in an Electrically Heated Tobacco Product. MARKUS NORDLUND, *Philip Morris Products S.A., Switzerland*

Philip Morris International is developing a range of products that have the potential to reduce individual risk and population harm compared with continued smoking. One of these products is the Electrically Heated Tobacco System (EHTS) (also referred to as the Tobacco Heating System 2.2), which is currently commercialized in more than 30 markets. During use, the patented EHTS heats a specifically designed tobacco product (Electrically Heated Tobacco Product (EHTP)) without combustion when inserted into the Holder (heating device). The EHTP contains a specially manufactured tobacco material in the form of a porous plug that undergoes a controlled heating process to release chemical compounds (present in the tobacco material) into vapors. As there is no combustion of the tobacco substrate, no smoke is formed, and the nicotine-containing respirable aerosol is instead formed with the help of an aerosol former (glycerol) added to the tobacco material.

The aim of this work was to numerically model the aerosol formation process for realistic operating conditions of the EHTS and for relevant gas-vapor mixture compositions measured in the generated EHTP aerosol. Chemical analysis of the EHTP aerosol showed that it consisted mostly of water, glycerol, and nicotine as well as other compounds at much lower concentrations. An extended Classical Nucleation Theory (CNT) for multicomponent gas-vapor mixtures was used to numerically model the aerosol formation taking place in the EHTP during use when operated in the Holder. Cases with and without glycerol present in the tobacco substrate were simulated to specifically investigate the role that glycerol plays during the aerosol formation process.

Results from the performed numerical simulations demonstrate that glycerol was the compound triggering aerosol formation under the simulated operating conditions of the EHTS and EHTP. Water and other compounds in the gas-vapor mixture were not able to reach supersaturation and therefore could not generate aerosol droplets from the multicomponent gas-vapor mixture at the operating conditions simulated. This implies that according to the extended CNT, an aerosol will only form under the tested operating conditions when there is an aerosol former, such as glycerol, present in the gas-vapor mixture.

6AM.4

A Multiscale Model for Evolving Multispecies Aerosol Deposition and Absorption in the Human Lung. Ravi Kannan, Z.J. Chen, ANDRZEJ PRZEKWAS, Florian Martin, Julia Hoeng, Arkadiusz Kuczaj, *CFD Research Corporation*

Computational fluid dynamics (CFD) models able to predict aerosol transport, evolution and deposition are useful in supporting and predicting in vitro and in vivo aerosol exposure and dosimetry results. Their ultimate goal of development and application would be to become integrated with in vitro bio-fluidics and in vivo physiological responses of the studied systems (e.g., CFD-PBPK linked approaches). The required level of sophistication of such mathematical models depends on the specific application. It is also often limited by the computational complexity of the respiratory system anatomy, and physiology. Detailed CFD aerosol deposition models are typically used for the trachea and upper bronchi, due to their high computational complexity and cost, while the approximate whole-lung models, such as the Typical Path Lung model, have issues concerning their application and accuracy.

To overcome the above mentioned barriers we have developed a novel multiscale computational model of human lung respiration physiology, including the inhalation of aerosols and their deposition on the airway walls followed by absorption and clearance via mucosal and alveolar barriers. In the conventional aerosol inhalation simulations, the airways are generally split into the upper airways and alveolar sections. Such “compartmental” models result in low-resolution results and the spatial resolution of the deposited aerosol cannot be accurately calculated. The foundation of the present multiscale model is the high-resolution anatomical geometry of a human entire respiratory tract from the mouth to the alveolar zone.

A two-step computational algorithm is used to predict the aerosol deposition. In the first step, high-fidelity 3D CFD simulations, on the adaptive Cartesian mesh, are performed to simulate air flows and transport of aerosol and gaseous compounds of the aerosol mixture. The spatial lung airway wall deposition patterns are computed and stored. In the second step, a novel, computationally efficient Quasi-3D (Q3D) airway wall barrier model is used to simplify the geometry and simulate both mucociliary and trans-mucosal absorption of the deposited compounds. The Q3D method preserves the 3D geometrical structure, delivering extremely accurate solutions and being approximately 25000 times faster than CFD methods. The Q3D lung airway model is then populated to around 15 generations (tracheo-bronchial limit). The alveolar region can be modeled using simplified bolus-type sacs matching the alveolar surface area, at the end of each bronchial leaf.

In the present multiscale model, the 3D CFD method is used to simulate the aerosol transport/deposition up to the first three airway generations. The Q3D model is then used to simulate aerosol transport/deposition in the distal airways. The resulting deposition is then used as the airway barrier model to simulate deposited aerosol mucociliary clearance and trans-mucosal absorption. The resulting mucociliary model is first implemented and validated against the experimental clearance results, involving non-absorbing radiolabeled particles. The paper presents selected validation results for the aerosol transport, deposition, and clearance in the lungs and comparison between previously published models and available experimental data.

6AM.5

Numerical Study of Flow Rate Effect on Hygroscopic Aerosol Transport and Deposition in a Basic Mouth-throat Airway with Realistic Wall Conditions. XIAOLE CHEN, Clement Kleinstreuer, Yu Feng, Tong Lu, Baobin Sun, Wenqi Zhong, *Southeast University*

Using an idealized mouth-throat (MT) airway as a test bed, simulations were carried out to investigate the impact of flow rate on hygroscopic aerosol transport and deposition (Longest et al., 2010). Specifically, a multi-layer structure, including the airway tissue and mucus layer, was constructed to simulate heat transfer across the MT boundary layer, i.e., conduction in the mucus layer and tissue, latent heat loss due to mucus evaporation, and convection over the mucus layer. The transport and deposition of the hygroscopic aerosols was simulated with a validated numerical program at three flow rates, i.e., 15 L/min, 30 L/min, and 60 L/min. The aerosols contained four components: water, ethanol, sodium chloride (NaCl), and fluorescein. The transition shear stress transport (SST) model and discrete phase model (DPM) were employed for the prediction of the air flow and aerosol transport, respectively. Modeling and validation of the aerosol deposition efficiency and aerosol-vapor interaction are discussed in our previous study (Chen et al., 2017).

The temperature of the tissue boundary toward the body surface side was set at 37 ˚C. The temperature of the mucus layer, which decides the saturation pressure of the water vapor, was determined by the heat transfer conditions, i.e., mucus evaporation, convection of the air and the conduction between the mucus layer and airway tissue. The air inhaled was assumed to be at room conditions, i.e., 26.7 ˚C and RH = 34%. For each flow rate, simulations with various initial aerosol diameters ranging from 2µm to 20µm were conducted to obtain the functional dependence between the aerosol deposition efficiency and the Stokes number.

The results are as follows:

1) Significant temperature gradients can be observed in the mucus-tissue region due to the latent heat loss of the mucus layer and convection along the air-mucus interface; especially under elevated flow rates.

2) The multi-component aerosols quickly evaporate in the relatively low humidity air, resulting in solid particles containing two components, i.e., NaCl and fluorescein.

3) Local regions of high RH (> 80%) almost disappear near the boundary at large inhalation flow rates, e.g., 60 L/min; hence, hygroscopic growth of NaCl and fluorescein particles is suppressed.

4) The growth ratios of the deposited and escaped aerosols both decrease with increasing flow rates.

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6AM.6

Understanding Particulate Matter Formation in CO2 Capture Plants using Molecular Dynamics Simulation. MEHDI AMOUEI TORKMAHALLEH, Mansurov Ulan, Dhawal Shah, *Chemical and Aerosol Research Team, Nazarbayev University*

Carbon capture has been proposed as a viable method that is capable to reduce CO2 emissions from power plants by 80 % to 90 %. The most advanced method in terms of industry is post-combustion CO2 capture (PCCC) using aqueous monoethanolamine (MEA) as a solvent. However, a major factor that precludes its widespread implementation is the high cost of the process, which is largely conditioned by substantial solvent losses during the process. These losses have been strongly linked to formation of aerosols or particulate matter (PM). Due to recent emergence of the issue, formation of aerosols (PM) has been an object of only few studies. Several efforts were made to model PM formation and behavior using commercial software such as ASPEN PLUS and MATLAB. Nevertheless, since these programs cannot model nucleation process, the attempts possess certain fundamental shortcomings. This original research aims to address the issue of PM formation in a PCCC absorption column at a molecular level using molecular dynamics simulation. The simulations were carried out using GROMACS software. Five different systems were considered including various configuration of components. Clustering effect of molecules has been observed in four systems out of five. Essentially, these molecular clusters are PM that emerge as a separate phase in the gas phase. Nucleation rate of the PM were in the order of 10-30 cm-3s-1 in all systems. In the systems with one condensable component PM formation was governed by saturation ratio. On the contrary, in the systems with several condensing components nucleation process was observed even if the gas phase was slightly sub-saturated. Special emphasize was made on interaction energies between participating components which drive the formation of PM. Inferred from simulation results, strong short-range attraction energy was reveled between water and CO2 and between water and MEA. Furthermore, radial distribution analyses were performed to examine the structure of formed PM. Based on the findings of the study certain practical suggestions were offered to decrease the formation rate of PM in a PCCC column.

6AM.7

Aerosol Formation and Growth in Amine-based CO2 Scrubber: Experiments and Numerical Simulation. DAVID I. A. DHANRAJ, Zhichao Li, Pratim Biswas, *Washington University in St. Louis*

The concerns owing to global warming and climate change have initiated significant efforts to reduce the concentration of atmospheric CO_2[1]. Post-combustion CO_2 capture using amine solvents is currently the key economical retrofit process for large power plants[2]. Amine loss is a primary challenge for amine-based CO_2 scrubbing technology considering its environmental and economic impacts. The presence of fine particles in flue gas is regarded as the major contributor of aerosolized amine emissions. Experiments using a lab-scale structured packing spray column were conducted to investigate the effects of inlet particle size distribution, gas flow rate and amine flow rate on the particle size distribution at the outlet. The results indicate that the total number concentration of particles with diameter in the range from 10 nm to 450 nm increased significantly after passing the scrubber. It was also seen that a small fraction of the particles larger than 1 µm was trapped in the scrubber. From these experiments, it can be inferred that increasing the number concentration of submicrometer particles and liquid flow rate could further increase the aerosol emission. Moreover, it is known that supersaturated amine in the vapor phase is the major contributor of aerosolized amine emissions. Amine vapor condenses on the fine particles and further grow by coagulation. In order to understand the processes that govern the formation and growth of particles, a discrete sectional model was used to simulate the relevant physical phenomena under industrially relevant operating conditions. Further experiments are performed to investigate the effects of amine and CO_2 concentration, operating temperature and pressure on aerosolization. These experiments and simulations provide insights for optimized design and operation strategy in order to minimize amine losses in a full-scale amine scrubber.

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6AM.8

A Field Dependent and Orientation Dependent Mobility Calculator: The Next Generation of Electrical Mobility Calculations. Behram Kapadia, Tianyang Wu, CARLOS LARRIBA-ANDALUZ, *IUPUI*

The ability to predict the electrical mobility of a charged entity from a molecular model is becoming of increasing interest as high resolution mobility measurements are more readily available. Most aerosol generated nanoparticles (and molecular ions and nanoclusters) are not spherical and require more than just a particle size to understand them or separate them. This asphericity may also be sought for as it may provide the particle with unique transport, optical and physical properties. Therefore, the commonly employed mobility diameter, i.e. the equivalent spherical diameter based on mobility measurements, while important in particle characterization, it is an ill conditioned parameter when dealing with molecules, nanocluster or particles with strikingly different aspect ratios. As such, we previously developed a very efficient parallelized state of the art algorithm, IMoS, that calculates collision cross sections (CCS) and mobilities of ion, clusters and nanoparticles within the free molecular regime from all-atom structures or coarse grain models. The CCS is equivalent to the mobility diameter but establishes the possibility of alluding to shape and orientation. It also has the advantage, unlike electrical mobility, that is not dependent a priori on the reduced mass of the gas-ion pair. For these reasons, it is the parameter of choice in IMoS to compare different nanoparticles/clusters.

The existing proposed algorithms however have their limitations. Among a few of such limitations, one can name 1) the calculations always assume that all orientations are equally probable ,2) that the mobility is independent of the electric field employed (true for E/N<<0), 3) that all atoms/coarse grained structures are assumed fixed which requires accommodation and reemission laws to be assumed and 4) that the ion/nanocluster has no rotational speed when the momentum exchange occurs.

Here we propose a novel MD/MonteCarlo algorithm that calculates the ion/nanoparticle as if it were in a real gas and subject to an arbitrary field in three dimensions. The ion/nanoparticle can freely rotate and its orientation, angular velocity and drift velocity are a function of the gas/ion collisions, the reduced mass, the strength of the field, and the position of the charges within the ion. It is the effect of the collisions and the particle orientation together with the electric field which now establishes the equilibrium drift velocity, preferred orientation, if any, and angular velocity. This equilibrium drift velocity, together with non-linearized theory establishes the relation between the field and the mobility which in turn yields the true mobility of the ion. This algorithm will not only provide new insights into mobility calculations never produced before but will also provide a unique understanding in multiple applications which involve charging efficiency, instrument sensitivity, diffusion losses or even collisional heating. The algorithm is parallelized and provides results within a reasonable amount of time. The code may also be extended out of the free molecular regime and into the transition regime when certain considerations are taken into account.

6AM.9

One Year Comparison of SOA Markers Modelling and Measurements: Seasonality and Gas/Particle Partitioning Evaluation. GRAZIA MARIA LANZAFAME, Deepchandra Srivastava, Florian Couvidat, Olivier Favez, Bertrand Bessagnet, Alexandre Albinet, *INERIS*

Secondary Organic Aerosols (SOA) account for a significant part of particulate matter (PM). Simulating their formation and fate remains challenging, since to date, air quality models usually underestimated them. SOA formation processes include multistep heterogeneous mechanisms, and their parametrizations involve several variables such as kinetic data and physical properties not well known. A better assessment of the SOA composition notably requires the understanding of the thermodynamic equilibrium of SOA compounds between the phases involved. This is usually done using either, theoretical, or experimental data. However, the validation of the modelling parametrizations developed must be done by comparison between measurement and modeling data. In this work, various key molecules, well known as SOA markers, have been modeled, using CHIMERE air quality model, through detailed formation pathways including the calculation of their gas/particle partitioning. Modelled concentration values have been compared to measurements of biogenic, (e.g. pinonic acid, pinic acid and MBTCA: α-pinene oxidation by-products), and anthropogenic (e.g. DHOPA: toluene SOA marker) SOA markers, performed on both, gaseous and particulate phases. Mechanisms have been developed based on data obtained from the Master Chemical Mechanism (NCAS, Universities of Leeds and York) and the scientific literature. The gas/particle partitioning has been calculated by using saturated vapor pressure and Henry’s constant values through the thermodynamic model SOAP. The gas phase chemistry has been simulated using MELCHIOR2. Biogenic emissions have been computed with the MEGAN 2.1 algorithm. The comparison has been done with SOA marker measurements performed for a one year period (2015) at the SIRTA sampling site (25 km SW from Paris city center). Filters and PUF (polyurethane foam) samples were collected every third day (24 h sampling) and then analysed by GC-MS after derivatization using native standards. The capacity of the model to reproduce seasonal variations of concentrations and the gas/particle partitioning (influenced by several parameters such as humidity and temperature) was evaluated.

6CC.1

Modification of the Versatile Aerosol Concentration Enrichment Factor System (VACES) for Cloud Condensation Nuclei Concentrator Purposes. CARMEN DAMETO DE ESPAÑA, Anna Wonaschuetz, Gerhard Steiner, Harald Schuh, Constantinos Sioutas, Regina Hitzenberger, *University of Vienna*

The activation of atmospheric aerosol particles into cloud droplets is fundamental for cloud formation. Cloud condensation nuclei (CCN), a subset of the atmospheric aerosol, constitute one of the largest uncertainties in estimating global climate change. The ability of atmospheric aerosol particles to act as CCN depends on many factors, including particle size, chemical composition, and meteorological conditions. To enlarge the knowledge on CCN, it is essential to understand the factors leading to CCN activation. For this purpose, a versatile aerosol concentrator enrichment factor system (VACES; Kim et al., 2001a; Kim et al., 2001b) has been modified to select CCN at different supersaturations. VACES allows for sampling of CCN particles without altering their chemical and physical properties. The redesigned VACES enriches CCN particle concentrations by first passing the intake flow to the saturator and then to the condenser. The activated particles are concentrated by an inertial virtual impactor, and then returned to their original size by diffusion drying. For the calibration, the saturator temperature was fixed at 50°C and the condenser temperature range was varied from 0°C to 40°C to obtain the activation curves for the different particle sizes. Knowing the activation dimeter, it was possible to calculate the supersaturation. Calibration results have also shown that CCN concentrations can be enriched by a factor of approx. 16. This correlates to the theoretical results. The theoretical enrichment factor is represented by the inlet main flow divided by the outlet minor flow which are 100 lpm and 5 lpm respectively.

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6CC.2

Method to Retrieve Cloud Condensation Nuclei Number Concentrations Using Multiwavelength Raman Lidar.

WANGSHU TAN, Chengcai Li, Yingli Yu, Chunsheng Zhao, *Peking University*

The uncertainties associated with the estimated climate forcing attributed to aerosol-cloud-interaction still span over a poorly constrained range. Determination of cloud condensation nuclei (CCN) number concentration (N_{CCN}) at cloud base is of central importance in aerosol-cloud-interaction observations. Ground-based lidar continuously provides useful vertical information about aerosols up to the cloud base and has potential to provide profiles of CCN-relevant particles. In this work, we propose a novel method to retrieve N_{CCN} by multiwavelength Raman lidar based on Mie theory and κ-Köhler theory using in situ aerosol measurement datasets. Variances of lidar-derived backscatter coefficient (β) and/or extinction coefficient (α) among different wavelengths, usually expressed as Ångström exponent, can describe the predominant size of aerosols. Enhancements of β and α with relative humidity in vertical direction are utilized to represent the hygroscopicity of aerosols. Results show that α contains more CCN-relevant information than β, and their enhancements with relative humidity are highly consistent with aerosol hygroscopicity. For a lower supersaturation ratio (0.1%), the retrieved error of our method is less than 20% only with β. For a higher supersaturation ratio (0.8%)， large systematic bias is found and the results significantly improve when α is adopted. We find that particles with diameters of 50-100nm dominate the retrieve bias at supersaturation ratio of 0.8%, because optical properties at lidar wavelengths are not sensitive to particles smaller than 100nm. This new method to retrieve N_{CCN} at cloud base directly from lidar observations would be able to provide long-term CCN data for aerosol-cloud-interaction studies.

6CC.3

CCN Activity of Secondary Organic Aerosol Largely Controlled by Molecular Weight. JIAN WANG, John Shilling, Jiumeng Liu, Alla Zelenyuk, David Bell, Markus Petters, Ryan Thalman, Fan Mei, Rahul Zaveri, Guangjie Zheng, *Brookhaven National Laboratory*

Aerosol particles strongly influence global climate by modifying the albedo and lifetime of clouds. An accurate assessment of the aerosol impact on climate requires the knowledge of the concentration of cloud condensation nuclei (CCN), a subset of aerosol particles that could activate and form cloud droplets in the atmosphere. Atmospheric particles often consist of hundreds, or even thousands of organic species, which collectively often dominate the composition of aerosol particles. As a result, CCN concentrations can be very sensitive to the hygroscopicity of the organics in the particles. Laboratory and field studies show organic hygroscopicity increases nearly linearly with the atomic O:C ratio (i.e., oxidation level). Such increase in hygroscopicity has long been thought a result of higher polarity and therefore increased water solubility for more oxygenated organics. In this study, we systematically characterized organic hygroscopicity of secondary organic aerosol (SOA) formed from representative precursors. We show that for the majority of SOA, organic hygroscopicity is mainly controlled by the molecular weight. Instead of increased water solubility, the increase of the organic hygroscopicity with O:C is to a large degree due to that (1) SOA formed from smaller VOC molecules tends to have lower molecular weight and higher O:C and (2) during oxidation, fragmentation produces organic molecules with lower molecular weight. A simple model of organic hygroscopicity based on molecular weight, O:C, and volatility is developed, and it successfully reproduces the variation of SOA κorg with O:C observed in the laboratory and field studies.

6CC.4

A Model Intercomparison of CCN-Limited Tenuous Clouds in the High Arctic. Robin Stevens, HAMISH GORDON, Katharina Loewe, Christopher Dearden, Antonios Dimitrelos, Anna Possner, Gesa Eirund, Tomi Raatikainen, Adrian Hill, Benjamin Shipway, Jonathan Wilkinson, Sami Romakkaniemi, Juha Tonttila, Ari Laaksonen, Hannele Korhonen, Paul Connolly, Ulrike Lohmann, Corinna Hoose, Annica Ekman, Ken Carslaw, Paul Field, *University of Leeds*

A decrease in Arctic sea ice extent and thickness has been observed within recent decades. Further decreases in Arctic sea ice extent are expected to increase the fluxes of aerosol and aerosol precursor gases as well as latent heat and sensible heat from the open ocean surface within the Arctic. Additionally, Arctic aerosol concentrations could be significantly impacted by changes in non-local aerosol sources and changes in the long-range transport of this aerosol, and increases in shipping traffic as the Arctic becomes seasonally ice-free. This increase in shipping traffic would also be expected to yield an increased demand for accurate weather forecasts over the Arctic region. However, it remains unclear whether the net effect of these changes in aerosol concentrations and surface fluxes would result in an increase or a decrease in cloud cover or drizzle precipitation. The changes in cloud properties could strongly influence the radiation budget in the Arctic, resulting in feedbacks on the rate of sea-ice loss. Arctic clouds remain poorly understood, and the current representation of these processes in global climate models is most likely insufficient to realistically simulate long-term changes.

In order to better understand the processes controlling Arctic clouds and their uncertainties in current models, we perform a model intercomparison of summertime high Arctic (> 80 N) clouds observed during the 2008 Arctic Summer Cloud Ocean Study (ASCOS) campaign, when observed cloud condensation nuclei (CCN) concentrations fell below 1 cm^{-3}. Previous analyses have suggested that at these low CCN concentrations the liquid water content (LWC) and radiative properties of the clouds are determined primarily by the CCN concentrations, conditions that have previously been referred to as the tenuous cloud regime. The intercomparison includes results from three large eddy simulation models (UCLALES-SALSA, COSMO-LES, and MIMICA) and three numerical weather prediction models (COSMO-NWP, WRF, and UM-CASIM).

We test the sensitivities of the model results to different treatments of cloud droplet activation, including prescribed cloud droplet number concentrations (CDNC) and diagnostic CCN activation based on either fixed aerosol concentrations or prognostic aerosol with in-cloud processing. We investigate the sensitivities of the model results to changes in these prescribed CDNC, fixed CCN, or prognostic CCN concentrations. Further, we examine the interaction of model sensitivity to CCN concentrations with changes in prescribed ice crystal number concentrations (ICNC). We also examine the interaction of model sensitivity to CCN concentrations with changes in surface heat and moisture fluxes due to a removal of sea-ice cover.

The results strongly support the hypothesis that the liquid water content of these clouds is CCN-limited. For the observed meteorological conditions, the cloud generally did not collapse when the CCN concentration was held constant at the relatively high CCN concentrations measured during the cloudy period, but the cloud thins or collapses as the CCN concentration is reduced. Our results also show that cooling of the sea-ice surface following cloud dissipation increases atmospheric stability near the surface, further suppressing cloud formation. This effect does not occur in simulations with a sea-ice-free surface.

There remains considerable diversity even in experiments with prescribed CDNCs and prescribed ICNCs. The sensitivity of mixed-phase Arctic cloud properties to changes in CDNC, and hence to changes in aerosol concentrations, depends on the representation of the cloud droplet size distribution within each model, which impacts on autoconversion rates. Our results therefore suggest that properly estimating aerosol–cloud interactions requires an appropriate treatment of the cloud droplet size distribution within models, as well as in-situ observations of hydrometeor size distributions to constrain them.

6CC.5

Marine Aerosol Cloud Activation. JURGITA OVADNEVAITE, Kirsten Fossum, Darius Ceburnis, Colin O'Dowd, *National University of Ireland Galway, Ireland*

Marine aerosol occurring in cloud condensation nucleus (CCN) sizes suggest that it may contribute notably to the CCN population, but further cloud droplet number concentration would strongly depend on the chemical aerosol composition and ambient (cloud) conditions, such as available water content, supersaturation and competition between the CCN of different composition (O'Dowd et al., 1999). Since the global importance of marine aerosol particles to the cloud formation postulated several decades ago, it has progressed from the evaluation of the nss-sulphate and sea salt effects to the acknowledgement of the significant role of organic aerosol (O'Dowd et al., 2004). It has been demonstrated that primary marine organics, despite its hydrophobic nature, can possess the high CCN activation efficiency, resulting in the efficient cloud formation (Ovadnevaite et al., 2011). Organic aerosol, ubiquitous in both clean and polluted atmosphere, can be present as a pure organic aerosol or and internally-mixed aerosol with other constituents such as sulphate and nitrate aerosol. The hygroscopicity of organic aerosol in sub-saturated humidity fields is typically less than most common salts found in the atmospheric aerosol; however, the ability of organic aerosol to activate cloud droplets is predicted to be greatly increased in supersaturated air due a lowering of the droplets surface tension, ultimately leading to more nuclei being activated at lower supersaturations (Facchini et al., 2000). While this phenomenon has been acknowledged for some time, we've demonstrated it in the real atmosphere (Ovadnevaite et al., 2017). Here we show the organic effect on primary and secondary marine aerosol activation to CCN. Results from two intensive measurement campaigns in the Eastern North Atlantic (Mace Head) and the Southern Ocean (PEGASO cruise) are presented here with the main focus on CCN dependence on aerosol chemical composition and, especially, origin and sources of marine organic. We investigate the activation of sea spray composed of the sea salt and externally mixed with nss-sulphate as well as the sea spray highly enriched in organics, stressing the importance of the latter to the formation of the cloud droplets. In addition, the organic effect on CCN activation of newly formed marine particles is investigated.

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6CC.6

The Role of Aerosol-Radiative Forcing on the Monsoon Trough Oscillations. RAJA BORAGAPU, Padmakumari B., R.S. Maheskumar, *Indian Institute of Tropical Meteorology (IITM), Pune, India*

The monsoon trough (MT) which forms as an elongated low pressure system over the northwestern part of South Asia during monsoon is part of the northward shifted Inter Tropical Convergence zone (ITCZ). Changes in the strength of MT can affect land-sea thermal contrast and further affect the advancement (progression) of the monsoon circulation. Any shift in the normal MT position causes shifts in the synoptic rain-bearing systems such as depressions leading to reduced rainfall over one region and enhanced over the other. The position of MT plays a major role as its southward shift leads to active and whereas northwards to the foothills of Himalayas causing break spells. On the other hand, aerosols through its interaction with radiation can increase the atmospheric stability and weaken the strength of the trough. Recent studies have shown a drying of the northern hemisphere mainly due to the aerosol induced cooling causing a southward shift in the climatic position of the convergence zone which may directly affect the total monsoon precipitation over the core monsoon zone in Central India. Therefore, using both observational and modelling approach this work attempts to understand the role of aerosol-radiation interactions in the MT oscillations. In the present study the impact of aerosols on MT characteristics and the resultant changes in the total precipitation during active and break conditions are explored and will be presented.

6CC.7

Overview of Fog Water Chemistry in Namibia during the AEROCLO-sA Campaign. Denise Napolitano, Stéphanie Rrossignol, Chiara Giorio, Roland Mushi, Gillian Maggs-Kölling, Barbara D'Anna, Bruno Coulomb, Jean-Luc Boudenne, Stuart J. Piketh, Andreas Namwoonde, Paola Formenti, Anne Monod, PIERRE HERCKES, *Arizona State University*

Namibia is an arid country where many rural and urban centers depend on ephemeral rivers for their water supply. These water sources are, however, limited and display seasonal salinization. Fog occurs along the coast and extends for up to 100 km inland, and has been considered for a long time as a source of drinking water. Fog is also a vital source of moisture for the endemic flora and fauna of the Namib Desert. However, due to the current change in climate and air quality, fog occurrence and composition, of crucial importance for the local ecosystems and populations, may be impacted.

The AErosol RadiatiOn and CLOuds in southern Africa (AEROCLO-sA) project investigated the interactions between aerosols, clouds and radiation fog in the South East Atlantic off the western coast of southern Africa. Within this framework fog and aerosol samples were collected in Henties Bay (Namibia), right at the Atlantic Ocean during an intensive campaign in September 2017. Eight fog events were sampled with two Caltech Active Stand Cloud Water Collectors (CASCC) operated in parallel, one stainless steel collector for organic matter analysis and one plastic collector for inorganic species characterization.

Fog samples were analyzed for pH, major ions, trace metals and organic carbon content (TOC and DOC). In addition, the fog samples were characterized by aerosol mass spectrometry (AMS-c-TOF-MS) and by optical spectroscopy including UV-VIS and 3D fluorimetric analysis. The results of the study will be presented and discussed relative to chemical data on local seawater and aerosol samples. Sea spray has been identified as the major source of many chemical species in these fogs. These results will be contrasted with fog chemistry observations at a more inland site in Namibia at the Gobabeb Research and Training Center. Here the marine impact is less dominant for many species.

6CC.8

Coastal Aerosol and Fog Microphysics in Atlantic Canada. RACHEL CHANG, Patrick Duplessis, Sean Hartery, Sonja Bhatia, Michael Wheeler, Annie Marie Macdonald, *Dalhousie University*

Fog reduces visibility, causing delays in transportation by land, sea and air. It is also a safety hazard that results in accidents and sometimes even death. Like cloud droplets, fog droplets form on cloud condensation nuclei, existing aerosol particles in the atmosphere that have the ability to activate into droplets. As such, fog provides a unique, in situ method of studying the process of aerosol activation. The interactions between aerosols and water vapour can determine the formation and persistence of fog, which makes fog forecasting challenging. Current parameterizations suffer notably from unresolved microphysical problems such as neglecting droplet concentration, which leads to large errors in droplet density predictions and therefore visibility. This study presents results from a fog study conducted on the eastern coast of Canada in Nova Scotia during the early summer of 2016. Observations of aerosol size distributions and chemical composition were conducted behind a ground-based counter flow virtual impactor, allowing the droplet residuals to be measured directly. Fog droplet size distributions, visibility and other meteorological variables were also measured at the same time. Aerosol and droplet microphysical parameters will be presented including the influence of air mass history on visibility. Preliminary results show that aerosol growth may be contributing to the dissipation of fog under some conditions, suggesting that despite the importance of dynamics on fog formation and dissipation, aerosols can also play an important role in the life cycle of fog.

6CC.9

Single Particle Measurements of Size and Mixing State of Black Carbon Particles Combined with Simplified κ-Köhler Theory Explains Their Droplet Activation Behaviour Observed in Fog and Clouds. MARTIN GYSEL, Ghislain Motos, Julia Schmale, Joel Corbin, Marco Zanatta, Robin Modini, Urs Baltensperger, *Paul Scherrer Institute*

Black carbon (BC) is an aerosol component, mainly emitted from anthropogenic sources, with peculiar properties. BC is the major light-absorbing component of atmospheric aerosols due to its high mass absorption coefficient (MAC), therefore causing substantial climate warming through aerosol-radiation interactions (ARI). BC in pure form is a poor cloud condensation nuclei (CCN) due to its insolubility, which makes wet deposition through the droplet nucleation pathway inefficient. Freshly emitted BC is often externally mixed, while it tends to acquire coatings during atmospheric aging processes. Such coatings can increase the MAC of BC. However, the corresponding effect on ARI may be partly compensated by reduced BC burdens as a consequence of better CCN activity and thus more efficient wet removal. In this study we address the droplet activation of BC in ambient fog and clouds, and assess whether BC activation can be predicted from measured BC properties.

A first field experiment was conducted in Zurich, Switzerland, an urban site where fog regularly occurs and where a mixture of fresh and aged BC is encountered. A second field experiment was conducted at the Jungfraujoch, Switzerland, a high-alpine site frequently exposed to clouds and with highly aged free tropospheric aerosol. Aerosol was sampled during fog/cloud periods using a total inlet to collect the aerosol as a whole (interstitial plus droplet residual particles) and an interstitial inlet to exclusively collect interstitial particles. Aerosol size distribution (mobility particle size spectrometer) as well as BC core size distribution and mixing state (single particle soot photometer, SP2) were measured behind both inlets along with complementary measurements.

Comparison of the measurements behind these two inlets makes it possible to compare the properties of particles that activated to cloud droplets with those remaining interstitial. The size distribution data provide the activation cut-off diameter representative of BC-free particles, from which the fog/cloud peak supersaturation is inferred. The SP2 provides, within its detection limits, the volume equivalent total particle and BC core diameters of BC-containing particles. This information combined with coating hygroscopicity was used as input for κ-Köhler theory to infer the critical supersaturation for CCN activation of BC on a single particle basis. Validity of these predictions was tested by comparing predicted critical supersaturations measured for BC particles behind the two inlets for fog/clouds with known peak supersaturation.

The fog in Zurich was characterized by large activation cut-off diameters of BC-free particles, which implies very low peak supersaturation. The BC particle activation agreed with predictions both qualitatively and quantitatively: activated fraction increased with increasing coating thickness for a fixed core size, the coating thickness at 50% activation decreased with increasing core size, and the observed dependence of the activation cut-off on size and mixing state of BC matched the theoretical line for the peak supersaturation in the fog events. Similar agreement between prediction and measurements was also found for the clouds at Jungfraujoch, though with more limited “data coverage” as clearly higher peak supersaturations shift the activation cut-off diameters towards the lower limits of detection of the SP2.

In conclusion, we achieved successful closure between observed droplet activation of BC and predictions based on measured size and mixing state for a range of peak supersaturations. This shows that assuming spherical core-shell morphology, which is implicitly done in both SP2 data analysis and κ-Köhler theory, describes activation behavior of atmospheric BC in good approximation. This validates application of κ-Köhler theory based on droplet activation in model simulations in which BC size and mixing state is available on a mass or volume basis.

6CD.1

Lung Capacity of Traffic Wardens Affected by Vehicular Pollution in Lahore, Pakistan. SAIMA YAQUB SHELLY, Husna Malik, Zulfiqar Ali, Farkhanda Manzoor, Sammuel Shahzad, Zaheer Ahmad Nasir, *Lahore College for Women University, 54600, Lahore, Pakistan*

Lahore was selected as the study site as it being the heart of Punjab and also the second most densely populated city of Pakistan and the 42nd most populous city in the world with a population of about 11 million people with a 2% growth rate leading to high number of increase in motorized vehicles in the last decade as well as the city attracting a higher number of commuters. It was the first city where the Traffic warden system were employed for the first time. A total recruitment of 3300 wardens were piloted in the past ten years.These wardens are alternated between areas of high, moderate and low traffic but being exposed to heavy vehicular pollutants has lead to health deterioration on a large scale. Long standing stressful duty hours increases the tendency to lose health faster than the common man. This study was conducted on randomly selected traffic wardens to check if the lung capacity of these physically well looking individuals has deteriorated with the passage of time along with pollution episodes at peak and non-peak hours in all ten towns of Lahore in both summer and winter seasons.

The lung capacity was measured for 500 cases under study by a digital portable spirometer MDX Spiro Tron. The values of FVC, FEV1 FEV1 predicted and FEV1/FVC were then used to categorize the individuals as per standards followed for Asians by National Institute for Health and Clinical Excellence (NICE) 2010 for severity of Chronic Obstructive Pulmonary Disease (COPD). Vehicular pollution data was monitored on ten sites marked throughout Lahore for sixteen hours each in both winters and summers for Temperature, Humidity, Nitrogen Dioxide (NO2), Carbon Monooxide (CO), $PM_{2.5}$ and PM_{10} with the help of Aeroquel portable monitor 500 for gases and GRADKO DC 1700 for particulate matter. The traffic density on the selected points was calculated by the number of vehicles crossing in a 24 hour time period, thus dividing the areas into Light, moderate and Heavy traffic density zones. The data obtained from the monitors was statistically analyzed by SPSS and reported.

The environmental data was collected during the summer and winter season for sixteen hours each with an interval of fifteen minutes. The data for wind speed and direction was obtained from the metrology department and depicted by synoptic charts denoting the level of pollution at the particular area when it was monitored.

It was observed that the temperature varied non-significantly between the towns whereas the humidity, CO level, NO_2 level, $PM_{2.5}$ and PM_{10} varied significantly between the towns. Significant correlation was observed between the varying seasons and temperature and $PM_{2.5}$ whereas as the humidity, CO and NO_2 correlated negatively with the seasonal changes. Temperature showed negative correlation with humidity and CO whereas NO_2 showed negative correlation with particulate matter value. Significant difference was observed for $PM_{2.5}$, PM_{10} and CO among towns with light and heavy traffic in both the summer and winter seasons.

As per the Kruskal-Wallis test the values of FEV1 and FEV1Pred also varied significantly for wardens of different towns in Lahore. Strong positive correlation was observed with high traffic density and low FVC and FEV1 values.

It is thus concluded from the study that the areas containing heavier load of traffic are more prone to emission to gases coming from those vehicles causing lung damage showed by decreased values of FEV1 and FEV1 predicted in individuals who have worked for longer periods of time and have been exposed the most thus concluding that long term exposure of vehicular emissions leads to lower lung capacities and higher disease symptoms.

6CD.2

Characterization of Electrophilic and Oxidative Potential of Atmospheric Carbonyls. JIN CHEN, Stacy Chen, Cody Cullen, C.M. Sabbir Ahmed, Ying-Hsuan Lin, *University of California, Riverside*

Ambient particulate matter (PM) is a prominent environmental risk factor associated with adverse human health effects such as asthma, cancer, and chronic obstructive pulmonary disease. PM represents a complex mixture consisting of numerous individual compounds, including carbonyls, which play a crucial role in atmospheric oxidation processes. Owing to the complex nature of atmospheric PM, currently a comprehensive understanding of molecular composition and toxicity of individual aerosol components is lacking. Sources of atmospheric carbonyls include direct emissions from cooking, cigarette smoke, and fuel combustion, or they can be generated through atmospheric degradation of volatile organic compound precursors. Upon exposure, some carbonyls such as unsaturated aldehydes are strong electrophiles that can react with thiol antioxidants and protein residues to induce inflammation and cellular oxidative stress. In this study, we calculate the global electrophilicity of atmospherically relevant carbonyls with computational chemistry approaches to estimate their chemical reactivity. Dithiothreitol (DTT) activity, a commonly used measure for PM oxidative potential, is assessed as a surrogate of biological activity. The reaction products of carbonyls with DTT are characterized using gas and liquid chromatography-mass spectrometry based methods to understand reaction pathways. The potential of using global electrophilicity as a descriptor for carbonyl reactivity in PM and toxicity screening will be discussed.

6CD.3: INVITED

Connecting the Dots in Nanotoxicology: From the Bio-Nano-Interface to Adverse Health Effects. Stefano Poggio, David Power, Hender Lopez, VLADIMIR LOBASKIN, *School of Physics, University College Dublin*

A definitive conclusion about the dangers associated with human or animal exposure to a particular airborne nanomaterial (NM) can currently be made upon complex and costly procedures including complete NM characterization with consequent careful and well-controlled in vivo experiments. A significant progress in the ability of the robust nanotoxicity prediction can be achieved using modern approaches based on the one hand on systems biology and on the other hand on statistical and other computational methods of analysis. Without the mechanistic understanding of the toxicity, one can only rely on statistical correlations between the NM properties and the toxicity endpoints. Thanks to the development of systemic approaches to analysis of biological systems (systems biology) and new methods of characterization and data generation in toxicology in the recent years, we are now in a position to make a step forward from the black-box-type statistical approaches and formulate a new paradigm in the toxicology – a mechanism-aware NM toxicity screening. We contend that the game-changing screening approach should be based on the detailed understanding of the response of the organism to exposure to NMs from the initial contact to the adverse outcome. To recover the mechanistic picture, we developed a research programme which includes in-vivo, in-vitro and in-silico studies to address main respiratory toxicity pathways, identify the mechanistic key events of the pathways, and relate them to interactions at bionano interface via careful post-uptake NM characterisation and molecular modelling, which is now funded through EU H2020 SmartNanoTox project.

In the SmartNanoTox project, we propose to construct a predictive model for gauging the toxicological and biological impacts of NMs using

- in vivo toxicity pathways for NMs that are of regulatory importance
- molecular initiating events and key events steering the toxicity pathways finally leading to an adverse outcome
- molecular mechanisms of NM involvement in these KEs
- structure and content of NM-biomolecule complexes after NM uptake.

The key step in the development of the smart screening approach is to combine the systems biology analysis of the responses of organisms to the NM exposure, resulting in a clear identification of the resulting pathways and key events, with the analysis of the whole chain of bionano interactions involving the NM inside the organisms.

The project team developed a number of innovative solutions to elucidate the key interactions involving airborn NMs. In this talk, I will present the project ideology and results to date.

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 686098.

6CD.4

The Impacts of Dust Storm Particles on Human Lung Cells - an Analysis at the Single Cell Level. KARIN ARDON-DRYER, Caroline Mock, Jose Reyes, Galit Lahav, *Department of Geosciences, Texas Tech University, Lubbock, T*

Aerosols particles (Natural and anthropogenic) are a key component of our atmosphere, their presence defines air quality levels and they can affect our health. Small particles penetrate into our lungs and this exposure can cause our lung cells to stress and in some cases leads to the death of the cells and to inflammation. During dust storm events there is an increase in particle concentration, many of them are breathable particles that can penetrate deep into our lungs. Exposure to dust particles can lead to respiratory problems, particularly for people with asthma. Therefore, during and after a dust storm event the number of people who are hospitalized with inflammation and respiratory problems increase. However, the exact mechanism that causes these health problems is still unclear. In this project, we are investigating the impacts that dust storm particles from different sources and of different concentrations (doses) have on human lung cells, performing a new and unique analysis at the single cell level. To accomplish this, each individual lung cell is continuously tracked after being exposed to dust particles. We monitor the behavior of the cell over time, identify the cells time of death and type of death (e.g. cell explosion). With this analysis, we can quantify cell death as a function of dust concertation (doses); to our surprise, an increase in cells death was not observed only as a function of an increase of dust concertation. In addition, we noticed that the way particles come in contact with cells, by sticking to or being engulfed by, and the interaction duration has an effect; cells that interact with dust particles for a longer period died earlier compared to cells with a shorter interaction period. These findings will help us to better understand the health-related consequences of exposure to dust storm events and serve as a baseline for when evaluating other aerosols.

6CD.5

Measuring the Real-Time Oxidative Potential of Ambient Particulate Matter Using an Online Mist Chamber System.

JOSEPH PUTHUSSERY, Chen Zhang, Vishal Verma, *University of Illinois Urbana-Champaign*

The oxidative potential (OP) of ambient particulate matter (PM) has been shown to be associated with various adverse health effects. Although there exist automated instruments which can measure the OP of ambient particles collected onto filters, there are both positive and negative artifacts associated with conventional filter sampling and their storage. Therefore, reactive oxygen species (ROS) activity measured on the archived filters is not representative of the real potential of ambient particles to generate ROS in the biological system on inhalation. To address this issue, we developed an automated online mist chamber (OMC) system to measure the hourly averaged OP of ambient PM using dithiothreitol (DTT) assay and tested it in the actual field conditions for over 50 days. The ambient particles were collected inside the mist chamber, and OP of the PM suspension was quantified using an automated instrument based on the DTT assay. The results from the online system correlated well ($R^2 > 0.80$) with conventional filter extraction method using both deionized water and methanol. The diurnal trend in the ambient particle OP during weekdays, measured by the online system showed a bi-modal trend with a peak during the morning period, followed by a broad peak (extending from 1 PM to 7 PM, but with a slight dip at 4 PM) during afternoon and early evening periods. We also conducted chemical speciation of the collected PM to link the diurnal variations in the concentrations of the redox active components (i.e., water soluble transition metals, organic carbon, water-soluble organic carbon, and elemental carbon) with the DTT activity. Based on our results, water-soluble Cu from non-exhaust emissions appear to be the major driver of the PM-induced OP during the daytime. Additionally, the secondary particles generated by the photochemical transformation of primary emissions were found to enhance the OP during the afternoon and evening periods. Future work in this direction aims to couple the OMC system to a comprehensive OP measuring instrument, which can measure both DTT consumption rate and hydroxyl radical (•OH) generation capability of aerosol particles using multiple assays (such as DTT assay and surrogate lung fluid assay).

6CD.6

Real-time Dosimetry for In-vitro Toxicological Studies of Engineered Nanoparticles (ENPs) at the Air-liquid Interface Using a Quartz Crystal Microbalance (QCM). Yaobo Ding, Patrick Weindl, Clara Wimmer, Paula Mayer, Tobias Krebs, OTMAR SCHMID, *Helmholtz Zentrum München, Germany*

Inhalation of engineered nanoparticles (ENPs), despite their unique physico-chemical properties compared to conventional materials, has been found to bear potential adverse effects on human health. In inhalation toxicology studies, direct air-to-cell exposure of ENP aerosols as possible with air-liquid interface (ALI) cell cultures provides a more physiologically-relevant platform to investigate their toxic effects, as compared to the traditional submerged cell culture systems. Moreover, the submerged cell exposures suffer from inaccurate control of the cell-delivered dose, which can be resolved by incorporating real-time dose measurement devices in ALI exposure systems.

In this study, we characterized the performances of the VITROCELL® CLOUD system (6- & 12-well model; VITROCELL Systems, Germany) for aerosolized ENP delivery to cells as well as the integrated QCM for measurement of the cell-delivered ENP dose. The system is equipped with a vibrating membrane nebulizer (Aeroneb Pro, Aerogen, Ireland) which generates aerosol droplets from a liquid suspension containing ENPs. As described by Lenz et al (2014) in the VITROCELL CLOUD system the aerosol droplets form a dense cloud, which utilizes cloud dynamics to rapidly (within 3 min) fill the exposure chamber, to uniformly mix the aerosol by vortex formation and to finally sediment the ENPs spatially uniform onto the transwell inserts containing the cells. A QCM is incorporated to monitor the cell-deposited dose.

A fluorescein solution was nebulized to investigate the uniformity and efficiency of aerosol deposition onto the cells cultured in transwell inserts as well as on the QCM. For the CLOUD 6 the deposition efficiency was 70.3%±1.9% and 63.5%±4.4% for inserts and the QCM, respectively, indicating no statistically significant difference. This was also the case for the CLOUD 12, but with slightly higher deposition efficiency (76-81%). These values are only weakly depended on the type of Aeroneb mesh nebulizers used. Out of six different nebulizers with varied output rates and droplet sizes, five resulted in the same deposition efficiency. Insert-to-insert variability was 4.4% and 6.0% for CLOUD 6 and CLOUD 12, respectively, within the range of nebulized volumes of ENP suspensions (50-400 µl). The QCM accuracy was 3.4% and 3.8% for CLOUD 6 and 12, respectively, as determined by using quantitative fluorescence spectroscopy on fluorescein as reference dosimetry method. The lower detection limit of the QCM was 500 and 170 ng/cm^2 for CLOUD 6 and CLOUD 12, respectively, which is above the onset dose for most types of ENPs. Finally, human lung epithelial cells (A549) were exposed to ZnO (JRC-NM110) nanoparticle aerosols and a dose-response relation was established from toxicological endpoints including cell viability (IC_{50}=ca. 0.5 cm^2/cm^2=4.2 µg/cm^2, membrane integrity and pro-inflammatory level.

Our results show that the VITROCELL-CLOUD systems can be used to deliver high dose rates of aerosolized ENPs (<1000 ng/cm^2/min) uniformly (<6% insert-insert variability) and efficiently to cells cultured at the air-liquid interface. Dose-response relationships can be readily determined with an integrated QCM providing real-time information on the cell-delivered ENP dose.

6CD.7

Application of Air-Liquid-Interface (ALI) Based In-Vitro Exposure of Human or Murine Lung Cells and Validation by Selected Animal Exposure Tests in the Framework of the HICE Consortium to Investigate Fresh and Aged Combustion Aerosols. RALF ZIMMERMANN, Maija-Riitta Hirvonen, Jorma Jokiniemi, Gunnar Dittmar, Jeroen Buters, Hanns Rudolf Paur, Carsten Weiß, Bert Buchholz, Tamara Kanashova, Sebastian Oeder, Marco Dilger, Tobias Krebs, Sven Ehlert, Thorsten Streibel, Juergen Schnelle-Kreis, Martin Sklorz, Stefanie Kasurinen, Sebastiano di Bucchianico, Johannes Passig, Jürgen Orasche, Mikko Happo, Hendryk Czech, Olli Sippula, Pasi Jalava, and further HICE co-workers (et al.), *Helmholtz Zentrum München and Rostock University*

Combustion aerosol emissions are responsible for acute and chronic health effects such as asthma exacerbation, heart-arrhythmia and heart-failure, lung cancer or COPD in humans. However, different combustion sources may have different health outcomes. Furthermore the effects may depend on the type of combustion compliance and can be mitigated/altered by abatement technologies. However, up to now only few links between aerosol chemical composition and biological effects have been established. Thus the relative toxicity of different combustion emissions needs to be determined experimentally. In the framework of the Virtual Helmholtz Institute-HICE (www.hice-vi.eu), physical and chemical properties of combustion emissions and their biological effects on lung cells (human epithelial cells: A549, BEAS2B and RAW/THP1 murine/human macrophages) are comprehensively analysed. For addressing the biological activity and toxicity of the aerosols, the lung cell-cultures were realistically exposed at the air-liquid interface (ALI) using 2 novel mobile automated ALI exposure-systems with 24 or 18 places for inserts with ca. 600.000 lung cells each (Vitrocell GmbH, Germany). The ALI systems are placed a mobile S2-bio safety laboratory (HICE MobiLab). One of the automated ALI systems is equipped with a newly developed exposure analysis system where the deposited mass, the particle size distribution (Topas GmbH, Germany) and the chemical composition is measured by mass spectrometry (Photonion GmbH). The cells are exposed with different moisturized com-bustion aerosols or clean air (reference). After 4h exposure biological effects were ana-lysed by multi-omics characterisation (transcriptomic, proteomic and metabolomics level) or assays for specific endpoints (viability, genotoxicity, cell integrity etc.). During all biological tests, the chemical composition and physical parameters of the emissions were thoroughly characterized (gases and particles). The acquired biological effects were comprehensively characterized and are put in context with the chemical and physical aerosol data (see e.g. Oeder et al., PLoSone 2015). For validation partly also animals (BL6 mice) are exposed in parallel to the ALI-exposures (RAW cells) and the macrophages from the broncheoalveolar lavage fluid (BALF) are subjected to molecular biological effects anaylsis as well. A first comparison of the effects from mice BALF (in-vivo) and RAW (in-vitro) for exposures with diluted exhaust from a Kubota diesel engine showed that immune response pathways are activated in both cases (in-vivo and in-vitro). Emissions from wood combustion (mansory heater, pellet burner and log wood stove, ship engines (heavy and light fuel oil), car engines (diesel, gasoline and ethanol fuels) were investigated by the ALI approach. Very recently lignite combustion and aging of wood and lignite aerosol emissions were investigated. The UV-light induced aging of the emission was performed in specially developed, high-throughput flow tube. In summary/conclusion observed biological response-strengths differ considerably for different combustion aerosol sources and are not well correlated to the deposited PM2.5-mass (i.e. partly also strong gas phase effects). This is suggesting large differences in the relative toxicity of the aerosol emissions from different combustion sources and fuel types. The aging experiments induce increased cytotoxicity, an effect which is currently deeper analyzed on the molecular biological level. In addition to adverse reactions also supposedly protective effects are observed. For example, the emission from a log-wood stove, exhibiting very high emission of soot, organics, PM2.5 are inducing only relatively mild acute effects in the ALI exposed cells, if compared to diesel or pellet burner emission. The high abundance of antioxidant compounds such polyphenols in the logwood stove-emissions may explain this counter-intuitive observation (Kanashova et al, J. Molec. Clin. Med., 2018). The latter findings are supported by detailed analyses of activated cellular response pathways (GO-term analysis), depicting regulation of pathways such as pro-inflammatory signaling, xenobiotic metabolism, phagocytosis or oxidative stress and findings from the selected animal exposure experiments.

6CD.8

Detection of Living Animal's Exhaled Breath Biomarker (dLABer) System. Haoxuan Chen, Xiangyu Zhang, Xinyue Li, Jing Li, MAOSHENG YAO, *Peking University*

In the past, toxicology studies are most offline, thus being not able to track the in situ responses of animals or humans to airborne pollutant exposure. Here, we report a system called dLABer that allows us to real-time monitor the breath-borne biomarkers. The system integrates living animals or humans, breath sampling, microfluidics, and biosensor. To test the dLABer, rats injected with PM were used as the subjects in this work. Our data showed that the dLABer were able to report IL-6 after 60 minutes from the breath sampling and can distinguish the different health effects caused by PM collected from different global cities based on the breath-borne IL-6 level. The results from the dLABer system were further validated using the ELISA for the air samples collected. In addition, the results from blood samples from the rats injected with different PM samples (the same mass) and also the DTT results agreed well with those from the dLABer system for breath-borne biomarker. In addition, video recordings also showed that rats exposed to PM with higher toxicity appeared to be less active, which was in line with the dLABer results. All the data (breath-borne, blood sera and DTT) suggested that the dLABer system can be used to real-time monitor breath-borne biomarkers. Results showed that the the dLABer were more sensitive than the traditional method ELISA, while the quantitative analysis capability of dLABer needs to be further improved. Here, we only tested the system for detecting biomarkers resulting from PM exposure, and in the future the dLABer system can be also used to detect the biomarkers resulting from the use of medications. Also, the system can be immediately used to monitor breath-borne biomarkers from humans in various scenarios. This work leads to a frontier method that is expected to revolutionize the pollutant health effects studies as well as many breath-borne disease diagnosis and studies.

6CD.9

Near-Roadway Effects on Expression of Autism Spectrum Disorder-Related Phenotypes. KEITH BEIN, Christopher Wallis, Xiao-San Luo, Elizabeth Berg, Michael Pride, Kelley Patten, Anthony Valenzuela, Eduardo Gonzalez, Jill Silverman, Pamela Lein, Anthony S. Wexler, *University of California Davis*

Recent epidemiological studies have linked traffic-related air pollution (TRAP) to increased risk of adverse neurodevelopmental outcomes, including psychomotor deficits, cognitive impairments, and autism spectrum disorders (ASD). In addition, in vivo and in vitro studies have shown that individual components of TRAP can alter neuroinflammation, alter neurotransmitter levels, and increase neurogenesis. However, TRAP exposures are challenging to reproduce in laboratory settings, and the mechanisms by which TRAP modulates neurodevelopment remain unclear. To address these issues, we exposed male and female Sprague-Dawley rats to real-time TRAP, using an exposure facility that samples air directly from a highway tunnel in the Bay Area of California used by both light- and heavy-duty vehicles. TRAP and filtered air (FA) PM samples were collected for 24 hours once every third day, and a subset of these were analyzed for particulate matter mass, organic and elemental carbon composition, and elemental composition. Gas phase samples were collected monthly on sorbents and analyzed for molecular organics. Rats were exposed to TRAP or filtered air (FA) from gestational day 15 to postnatal day 50. Following exposure, animals were assessed for ASD-relevant behavioral phenotypes and markers of brain cell development. The latter included microglial infiltration, reactive astrogliosis, and neurogenesis as assessed using immunohistochemistry, and ventricular volume and extra-cerebral volume as determined using magnetic resonance imaging (MRI). These data suggest that exposure of the developing brain to TRAP disrupts normal neurodevelopment.

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6IB.1: KEYNOTE
Mechanistic Modeling of Pathogen Transmission. LYDIA BOUROUIBA, *Massachusetts Institute of Technology*

The mechanisms governing the transfer of pathogens between infected and non-infected members of a population are critical in shaping the outcome of an epidemic. Despite major efforts aimed at the mathematical modeling and mitigation of infectious diseases, the fundamental mechanisms of pathogen spreading for most infectious diseases remain poorly understood. Drawing upon clinical or field data, fluid experiments and multi-scale mathematical modeling I will discuss the dynamics of transmission of various pathogens through the lens of fundamental fluid fragmentation.

6IB.3

Aerosol Particle Emission and Super-emission during Human Speech. SIMA ASADI, Anthony S. Wexler, Christopher Cappa, Nicole M. Bouvier, Santiago Barreda, William D. Ristenpart, *University of California Davis*

The traditional emphasis for airborne disease transmission has been on coughing and sneezing, which are dramatic expiratory events that yield easily visible droplets. Nonetheless, it has long been known that normal speech also yields expiratory aerosol particles. Recent research indicates that, compared to coughing, speech can actually release even larger quantities of such particles that are too small to see by eye, but are large enough to carry a variety of communicable respiratory pathogens. Here we show that the rate of aerosol particle emission during normal human speech is strongly correlated with the loudness (amplitude) of vocalization, ranging from approximately 1 particle per second for soft speech to over 50 particles per second at high amplitudes, regardless of the language spoken (English, Spanish, Mandarin, or Arabic). Furthermore, a small fraction of individuals behave as “superemitters,” consistently releasing an order of magnitude more aerosol particles than their peers. The results suggest that individual speech patterns could affect the probability of airborne respiratory disease transmission, and also help explain the existence of “superspreaders” who are disproportionately responsible for outbreaks of airborne infectious disease.

6IB.4

Novel Method for Identification of Airborne Transmission Using Molecular Epidemiology. Donald Milton, Daniel J. Nasko, TODD TREANGEN, *University of Maryland*

We subjected three pairs of fine-aerosol and NP swab samples (from our archive of 188 paired samples with detectable viral RNA in aerosol samples) to deep sequencing as described below (except that for exploratory analysis we used 20 samples per MiSeq lane). This preliminary sequencing effort tested the feasibility of the proposed work by selecting aerosol samples covering the range of measured fine-aerosol viral RNA content from ~10^3 to 10^7 copies per 1 mL. We achieved an average read depth of 15,000X per sample (ranging from 12,000X to 20,000X). All variants with p-value < 0.05 and at allele frequency >=2% were considered true variants; the rest were discarded as putative false positives. This cutoff level is consistent with those used in several recent analyses of the transmission bottleneck for influenza and high enough to exclude variants that would be unlikely to be transmitted through a bottleneck of 100. For each of the six samples sequenced for the feasibility study (three pairs of NP swab and aerosol), we identified the set of single nucleotide polymorphisms (SNPs) unique to one sample compared across all samples, unique to each member of the pair within the pair. The number of variants found in one but not both members of each pair ranged from 20 to 147 with no shared variants; thus, Jaccard similarity coefficients were zero. Phylogenetic analysis demonstrated that two of the paired samples were very closely related with consensus sequences differing by fewer than 10 SNPs. The third subject's consensus sequences from two sites differed by 73 SNPs, raising a question of two separate infection events at different sites. Overall, these preliminary data show that we can detect and distinguish variants and consensus sequences from the NP swab and the fine particle aerosol samples. If these results are confirmed by sequencing of additional samples, we will be able to establish that viral populations in the NP swabs and aerosol samples are independent. Success with these few samples suggests that we will be able to use the differences in consensus sequence and variant populations as markers of whether transmitted virus between two cases was from viral aerosol or a nasal source.

6IB.5

Foot-and-Mouth Disease Aerosols: Past and Future Perspectives. CLAIRE COLENUTT, Noel Nelson, Emma Brown, Simon Gubbins, *The Pirbright Institute*

Foot-and-mouth disease virus (FMDV) is a globally important pathogen of cloven hooved animals, which can be transmitted via numerous routes. Transmission through direct contact with infected animals is the most common route of spread of FMDV, but can be prevented by implementation of control measures, such as culling and movement restrictions. The role of indirect contact and fomite transmission is less well understood and more complex to apply effective control measures.

The ability of the FMDV to be transported long distances in aerosols given appropriate epidemiological and meteorological conditions has generated interest in understanding how the virus behaves in aerosol form and how this impacts on the overall epidemiology of the disease. Using empirical data generated in experiments, airborne spread of the virus can be modelled, alongside other transmission routes, to inform surveillance efforts and control measures in the event of an outbreak.

Here, we present a summary of research into FMDV aerosols. This covers work ranging from determining patterns of excretion of airborne virus from key susceptible livestock species, to demonstrating FMDV aerosols as a viable route of transmission. Numerous air sampling devices have been trialled for use in FMDV research, although the ideal qualities of equipment vary as to the research question being approached.

Existing research has provided answers to fundamental questions, but new tools and approaches are now required to be able to probe deeper into the aerobiology of FMDV. The development of operational tools to aid surveillance efforts in the event of an outbreak is a particular goal for future work. Research into FMDV aerosols is complicated by the need to carry out all experimental work under high containment. Ideal research methods and tools would incorporate the necessary protocols for containment and rigorous disinfection of equipment.

6IB.6

Stability of Variant H1 Subtype Influenza Viruses in Aged Aerosols and Their Infectivity in the Ferret Model. JOANNA PULIT-PENALOZA, Jessica Belser, Terrence Tumpey, Taronna Maines, *Centers for Disease Control and Prevention*

The relative importance of influenza virus transmission via aerosol inhalation is not fully understood and the subject of some debate. Detection of influenza virus RNA in the air collected directly from infected individuals and from contaminated spaces occupied by infected individuals, as well as mathematical modeling studies, suggest that aerosol transmission may represent a critical mode of seasonal influenza virus transmission in humans. Prototypical lab influenza viruses were shown decades ago to maintain viability in aerosols; however, there is a paucity of data available on currently circulating influenza viruses that significantly differ genetically and antigenically from their predecessors. In this study, we modified a previously established aerosol exposure system to assess stability in aerosols of four swine-origin variant H1 influenza viruses, isolated from humans in recent years, and a human seasonal influenza virus. Following nebulization of influenza virus into the primary exposure chamber, airflow through the chamber was interrupted to allow aerosol particles to age under still air conditions at 23-24°C and 45-55% relative humidity. Time-dependent loss of infectious virus was observed as evidenced by higher total viral RNA levels over total viable virus. Among the H1 viruses tested here, stability in aerosols correlated with transmissibility between ferrets, the gold standard animal model of influenza infections in humans. The influenza viruses that were transmissible through the air with 100% efficiency among ferrets displayed higher stability in aerosols than the viruses that transmitted with lower efficiency. Virus-laden aerosols aged for 15 or 30 min were able to productively infect ferrets at low doses, despite diminished viral viability compared with aerosols that were generated immediately prior to ferret exposure. Collectively, these data underscore the high infectivity of influenza viruses in aerosols, and support the need for continued refinement and innovation of laboratory methods to investigate mammalian exposure to inhaled pathogens. The results of this study further our understanding of the public health threat posed by novel influenza viruses as they continue to cross the species barrier to cause human infections.

6IB.7

Influenza Virus Maintains Infectivity in Droplets and Aerosols Independent of Relative Humidity. Karen Kormuth, Kaisen Lin, Aaron Prussin II, Eric Vejerano, Andrea Tiwari, Steve Cox, Mike Myerburg, Seema Lakdawala, LINSEY MARR, *Virginia Tech*

Previous studies have suggested that humidity contributes to the seasonality of influenza because the virus appears to survive better in droplets and aerosols under cold, dry conditions. However, there are conflicting findings about virus viability across the full range of relative humidities (RHs). Our objective is to determine the relationship between RH and influenza virus viability in droplets and aerosols of physiologically realistic composition. We exposed a circulating strain of influenza virus (2009 pandemic H1N1) in both stationary droplets and suspended aerosols to RHs ranging from 23% to 98%. The virus was prepared in a 1:10 mixture of human bronchial epithelial extracellular material and L-15 media. Over the 1-hour exposure period, the virus did not lose infectivity at any of the RHs tested. Our data suggest, for the first time, that influenza viruses remain highly stable and infectious in aerosols, independent of RH. When the extracellular material was heat-treated to denature proteins, the virus did not survive as well, particularly at RHs around 50%, as seen in prior studies. A parallel experiment with the enveloped bacteriophage Phi6 showed that the human bronchial epithelial extracellular matrix conferred a protective effect on this virus, too, and confirmed that viability in stationary droplets was similar to that in suspended aerosols. These results have significant implications for understanding the mechanisms of transmission of influenza and its seasonality.

6IB.8

Aerosol and Surface Sampling for a Novel H7N2 Influenza A Virus at a New York City Feline Quarantine Facility.

WILLIAM LINDSLEY, Francoise Blachere, Angela M. Weber, Donald Beezhold, Robert Thewlis, Kenneth R. Mead, John Noti, *National Institute for Occupational Safety and Health*

Influenza is of tremendous concern to the public health community because of the potential for new strains of the virus to cause a severe pandemic. In December 2016, an outbreak of a novel avian-lineage H7N2 influenza A virus was detected among cats in three animal shelters in New York City. H7N2 influenza had never been previously reported in cats, and further investigation found that at least one case of cat-to-human transmission to a veterinary staff member had occurred. To contain the outbreak, 500 cats that were potentially exposed to the virus were moved to a temporary feline quarantine facility and infection control measures were implemented.

In order to better understand the possible transmission pathways of the virus and the occupational exposure risk for animal shelter workers, the National Institute for Occupational Safety and Health (NIOSH) conducted aerosol and surface sampling in the quarantine facility. The quarantine facility was housed in a two-story warehouse with recirculating air heaters and natural ventilation. The animal isolation zone had a floor area of approximately 220 m2 (7800 ft2) and a ceiling height of approximately 3.7 m (12 feet). During sampling, the interior temperature was 18°C and the relative humidity was 25%.

Twenty aerosol samples were collected using NIOSH two-stage cyclone aerosol samplers with a 3.5 liter/min sampling rate for 4-5 hours. The NIOSH sampler separates aerosol particles into three size fractions (≥4 µm, 1 to 4 µm, and ≤1 µm) and conforms to the ACGIH/ISO criteria for respirable particle sampling. Sixteen aerosol samples were collected within the isolation zone, and all of these samples were positive for the H7N2 virus by RT-PCR. The mean concentration of airborne H7N2 influenza virus was 5810 viral copies/m3 of air (SD 4230). Seventy-one percent of the virus was detected in particles ≥4 µm, while 28% was found in 1-4 µm particles, and 1.4% in ≤1 µm particles. Influenza was not detected in 4 aerosol samples collected outside the isolation zone.

Thirteen aerosol samples were collected in the isolation zone using SKC BioSamplers at 12.5 liters/minute for 60 minutes. The SKC BioSampler collects particles into a liquid viral transport media, which helps preserve the viability of the virus. Sterile distilled water was added to the BioSamplers every 15 minutes as needed to replace water lost due to evaporation. Twelve of these aerosol samples were positive for H7N2 influenza by RT-PCR, with a mean airborne concentration of 3260 viral copies/m3 of air (SD 1830). Viable airborne influenza virus was detected in 6 samples.

Thirty-one surface samples were collected using sterile nylon-flocked swabs moistened with viral transport media. Of the 22 surface swabs taken in the isolation zone, 17 were positive for H7N2 influenza by RT-PCR, with a mean of 1030 viral copies/sample (SD 1890). Viable influenza virus was detected in 5 surface samples. Nine surface swabs were collected outside of the isolation zone, none of which were positive for influenza.

The results of this study show that airborne and surface H7N2 influenza virus were pervasive throughout the isolation zone of the quarantine facility, which suggests that airborne, droplet and contact transmission were all potential pathways for the spread of the virus. These results also indicate that occupational exposures to the virus could occur by all three routes, which helps inform decisions about appropriate protective measures for the animal care workers. Finally, this study illustrates the need for a prompt risk assessment of any newly-emerging pathogenic microorganism to help control disease transmission, prevent occupational exposures, and protect the public health.

6IB.9

Exposure of Cynomolgus Macaques To Small Particle Aerosols Containing H5N1 Avian Influenza Triggers Rapid, Lethal Acute Respiratory Distress Syndrome. DOUGLAS REED, Elizabeth Wonderlich, Katherine O' Malley, Jennifer Bowling, Amy Hartman, Jonathan Carney, Charles Scanga, Daniel Perez, Simon Barratt-Boyes, *University of Pittsburgh*

Avian influenza viruses including H5N1 and H7N9 can trigger severe, often fatal disease in humans. Severe viral pneumonia caused by H5N1 or H7N9 is thought to be a lower respiratory tract disease whereas seasonal influenza is a upper respiratory tract disease. Intratracheal and/or intranasal inoculation of virus only rarely results in severe, lethal disease in cynomolgus macaques. We developed a system for aerosol exposure of macaques to a highly pathogenic avian influenza virus, H5N1 (A/Vietnam/1203/2004). Macaques were exposed in a head-only chamber side a class III biological safety cabinet in the regional biocontainment laboratory at ABSL-3+. Aerosols were generated with an Aeroneb vibrating mesh nebulizer (Aerogen, Deerfield, IL) controlled by the AeroMP aerosol exposure system (Biaera Technologies, Hagerstown, MD). Aerosol sampling was accomplished using an all-glass impinger (Ace Glass, Vineland, NJ) and Aerodynamic Particle Sizer (TSi, Inc, Shoreview, MD). Initial studies prior to macaque exposures demonstrated that for virus aerosols the Aeroneb was consistently superior to the Collison 3-jet as measured by spray factor. Relative to fluorescein, there was little or no loss of influenza with the Aeroneb compared to a >90% loss of influenza with the Collison 3-jet nebulizer. Particle sizes generated by the Aeroneb were in the respirable range that would reach the deep lung. Within 18 hours of infection, macaques were febrile and there were significant changes in respiratory function which worsened on days 2 and 3. PET/CT imaging at 48 hours revealed a considerable inflammatory response in the lung. Mean time to death was 72 hours post-infection. Pathological and clinical findings all suggest the cause of death is acute respiratory distress syndrome (ARDS) which strongly represents what is seen in humans. Even at aerosol doses 10-fold lower than had previously been reported for other routes of inoculation, the disease was rapid and fatal in macaques. This new nonhuman primate model will be useful for developing and testing new vaccine or therapeutic approaches to treat severe human disease caused by avian influenza viruses.

6IM.1

Detection of Polyaromatic Hydrocarbons, as Well as Positive and Negative Inorganic Ions from the Same, Individual Particle. Johannes Passig, Julian Schade, Robert Irsig, Sven Ehlert, Martin Sklorz, RALF ZIMMERMANN, *Helmholtz Zentrum Munich and Rostock University*

Air pollution represents the largest environmental risk to health worldwide. Herein inhalation of polyaromatic hydrocarbons (PAHs) is an established cause of morbidity and mortality, but little is known about their detailed distribution in ambient particulate matter (PM). These details, e.g. the PAHs mixing state, are crucial for potential effects since PAHs may be equally distributed over a large particle ensemble or could be confined to a specific particle sub-type with high concentration producing strong local effects in the lung. Furthermore, PAHs are considered for taking an active role in secondary aerosol formation. As a consequence, novel aerosol characterization techniques that address PAHs on a single particle basis while providing information on their potential source are highly desired.

On-line techniques for individual particle profiling typically base on the Aerosol Time-of-Flight (ATOF) technique, which applies laser-desorption/ionization (LDI) of individual particles in the ion source of a bipolar mass spectrometer. Particle LDI is often limited to refractory inorganic compounds, while particle-bound molecules are typically fragmented. Approaches targeting on PAHs could not preserve the normal LDI-information on the inorganic bulk composition. Recently, we were able to complement the PAH information by positive inorganic ions from LDI using a complex laser ionization scheme. Here we present a route to obtain the full LDI information of both positive and negative inorganic ions in combination with PAHs. Thus, a conventional source apportionment that bases on ions of either charge can be combined with a fully-fledged PAH mass spectrum of individual particles.

6IM.2

Performance of a New VOCUS-PTRTOF for Detecting Volatile-, Semi-Volatile and Low-Volatile Organic Compounds.

PEKKA RANTALA, Matthieu Riva, Jordan Krechmer, Yanjun Zhang, Olga Garmash, Liine Heikkinen, Felipe Lopez-Hilfiker, Otso Peräkyla, Yonghong Wang, Mikael Ehn, *University of Helsinki*

Volatile organic compounds (VOCs) have a major impact on aerosol particle formation in the atmosphere. The development of new instruments – mainly mass spectrometers –, has brought new information to better understand the process chain from VOC emissions to oxidized compounds and condensation onto aerosol particles. However, to quantify each step of these chemical and physical processes, it is crucial to measure not only VOCs but also the wide variety of oxidation products from low to highly oxygenated molecules (HOMs).

Usually, the gas-phase measurements have been conducted using mass spectrometry with several different inlet designs to fill all the gaps between VOCs and HOMs. However, this is problematic in many ways. Calibrating all the instruments in a comprehensive way has remained especially challenging. In addition, operating several instruments is laborious, and availability of space and electricity can also be limited in remote locations. Therefore, instruments that can measure a wider range of compounds would be of great interest.

VOCUS PTR-TOF (proton transfer reaction time-of-flight mass spectrometer, TOFWERK AG/Aerodyne Research, Inc.) is a new instrument for detecting volatile organic compounds. The instrument is based on a new PTR-inlet design with sub-ppt detection limits. In December 2017, we organized a laboratory campaign, in which we explored the capability of the VOCUS to simultaneously measure α-pinene oxidation products generated from the ozonolysis of α-pinene under a wide variety of experimental conditions. Chemical characterization of gas-phase products was compared to several other types of chemical ionization mass spectrometers.

While data processing is still under way, first results indicate sensitive detection of the precursor and oxidized monomers (e.g. $C_{10}H_xO_{<8}$). For more oxidized products and/or dimers, the VOCUS either cannot measure these compounds or the instrument must be tuned more carefully to optimize its performance for these molecules.

6IM.3

Factors Affecting the Detection of Fine Particles by Secondary Nanoelectropray Ionization High Resolution Mass Spectrometry. Dandan Jin, Anthony S. Wexler, Jiafa Zeng, Man Nin Chan, Zhen Zhou, Yong Jie Li, XUE LI, *Jinan University*

Chemical characterization of aerosol particles at a molecular level is crucial to obtain a better understanding of their impacts on atmospheric chemistry, global climate and human health. Real-time mass spectrometry (MS) based methods have attracted attention due to their merits, which include high time resolution (seconds to minutes), minimization of artifacts resulted from condensation/evaporation during sample pretreatment and avoidance of time-consuming sample pretreatment. Recent studies have indicated that a soft ionization MS technique, secondary/extractive electrospray ionization MS (SESI/EESI-MS) is a promising alternative for the characterization of organic aerosol particles at the molecular level. However, ionization of particle-phase compounds in SESI is quite different from that in gas phase and the procedure is more complicated. Thus, investigations are needed into relevant SESI-MS operating parameters that improve sensitivity, selectivity and user-friendliness. In this study, a secondary nano-electrospray ionization (Sec-nanoESI) source was constructed and coupled with a high resolution quadrupole Orbitrap mass spectrometer (HRMS) for measurements of aerosol phase tartaric acid. Factors affecting the detection of TA particles using Sec-nanoESI-HRMS are systematically investigated and discussed. Temperature of the ion transport tubing (ITT) has the most pronounced impact on ion signal intensity, which may be ascribed to more efficient desolvation and ionization; normalized collision energy (NCE) applied in MS/MS measurement is also a parameter to be tuned to obtain the optimal fragment for quantitative analysis with higher specificity and sensitivity. By using the developed method, high sensitivity (a detection limit of 0.078 μg/m3) and a wide linear range (0–1.686 μg/m^3) of TA detection was achieved, providing a proof-of-concept demonstration for our Sec-nanoESI-HRMS in real-time measurements of atmospheric particulate organic matter.

6IM.4

Mechanistic Insights into the Ionization of Airborne Nanoparticles via Droplet Assisted Ionization (DAI). DEVAN E. KERECMAN, Michael J. Apsokardu, Murray Johnston, *University of Delaware*

Online methods for molecular analysis of secondary organic aerosol have the potential for fast time resolution measurements while consuming a minimal amount of sample. Understanding the ionization mechanisms behind these techniques allows for their optimization and successful application. Our group has developed an online technique, Droplet Assisted Ionization (DAI), where liquid droplets are sampled through a heated capillary into the mass spectrometer. The solvent medium assists formation of ions from analytes in the droplet, but the ionization mechanism and corresponding experimental conditions required for optimum detection are poorly understood. Current theories regarding the mechanism of DAI suggest an ionization process similar to electrospray ionization, but do not clearly explain how the initial charge is induced on the droplet. The work described here offers insight into the ion formation process by using two peptide-based aerosols, bradykinin and angiotensin II, as well as a polymer-based aerosol, poly(propylene)-glycol. The ion signal is found to increase linearly with aerosol mass concentration. There is no particle size dependence other than the fact that a large particle has more mass (and gives a correspondingly higher signal) than a small particle. A detectable signal is obtained for an aerosol mass flow into the inlet of about 80 pg/s. For the peptide aerosols, water is crucial for ionization. Drying an aqueous aerosol to remove water decreases the analyte signal intensity by 2-3 orders of magnitude. A similar reduction in signal intensity is observed when drying droplets composed of 50/50 water/acetonitrile solvent. Inlet temperature has a smaller but still important effect: signals are about an order of magnitude higher for inlet temperatures above 500 C than for lower temperatures. We find that additives, which increase the ion yield in a conventional inlet ionization experiment (e.g. 3-nitrobenzonitrile in Matrix Assisted Ionization, MAI), have little or no effect in DAI. This result suggests that such additives in a conventional experiment serve the purpose to create an aerosol, which is not needed in our work since aerosols are already being analyzed. The results of this study elucidate the conditions for efficient analysis of secondary organic aerosol by DAI.

6IM.5

Utilizing Bromide Chemical Ionization Technique in Detecting Oxidized Organic Compounds. Xucheng He, YEE JUN THAM, Siddharth Iyer, Mikko Sipilä, Matti Rissanen, *University of Helsinki*

Highly oxidized multifunctional (HOM) compounds have been found to play a crucial role in the atmospheric aerosol formation[1] and yet, direct measurement of many of these oxidized organics in the ambient air has remained challenging. Mass spectrometric methods using nitrate ionization[1], iodide ionization[2], and protonated water clusters[3] have been recently applied for direct detection of highly oxidized organic molecules in laboratory and field studies.

In this work, we explore the possibility of using a bromide chemical ionization technique to detect oxidized organic compounds. A Chemical Ionization Atmospheric Pressure interface Time-Of-Flight (CI-APi-ToF) was optimized to operate using bromide as the reagent ion. A series of test runs and calibrations for the instrument were conducted in our laboratory and scientific experiments were carried out in the CLOUD chamber in CERN. The results show that the bromide chemical ionization technique can detect a broad range of oxidation products; in form of $C_xH_yO_z^-$ and/or $(C_xH_yO_z)Br^-$ from oxidation of alpha-pinene (by O_3 and OH) under various temperature conditions. An interesting observation is that the hydrogen numbers in most of the deprotonated/dehydroxylated organic ions are odd, indicating that the bromide ionization process has stripped off one hydrogen atom (deprotonation) or potentially together with an oxygen atom (dehydroxylation) from the neutral molecules, which were not widely observed with the nitrate ionization method. The detected oxidized organic ions from bromide CIMS were compared with HOM species detected by a nitrate CIMS to examine if they present the same molecular structure or not under different experimental conditions (i.e. with or without NO_x). Another question that arose from our observations is whether the deprotonated/dehydroxylated ions and the organic-bromide cluster ions represent the same oxidation products, but are charged by a different mechanism (i.e., clustering vs charge transfer reaction), or are they compounds with same chemical formula but with a different chemical structure, i.e., are they isomeric products.

Overall, our study shows that the bromide ionization technique can detect a wider range of oxidized organic species, especially lower-oxidized species, compared to the nitrate CIMS. The comparison between the two ionization methods also helped shed light on the molecular structure of the detected oxidized organic species.

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6IM.6

Chemical Composition of Atmospheric Ion Clusters Measured with the New ioniAPi-TOF. Markus Leiminger, Paul Mutschlechner, Daniel Gunsch, Arttu Ylisirniö, Stefan Feil, Alfons Jordan, Siegfried Schobesberger, Armin Hansel, GERHARD STEINER, *University of Innsbruck*

The Atmospheric-Pressure-interface developed by Tofwerk AG, Thun (Switzerland), for Time-of-Flight mass spectrometry (APi-TOF MS) is a technique especially suited to the detection of very low number concentrations of ions (a few hundred per cubic centimetre) in the atmosphere for subsequent identification of their chemical composition.

The Atmospheric-Pressure-interface of the new ioniAPi-TOF from Ionicon Analytik GmbH, consists of two hexapole ion guides, followed by an Einzel-lens system and an orthogonal acceleration time-of-flight mass analyser. The mass resolution m/Δm of the instrument is larger than 2000 (FWHM) with a total ion transmission of about 1%. The hexapoles used in this instrument allow for an almost constant ion transmission over a wider mass range than observed before. In the context of atmospheric ion clusters, this means that not only high-mass cluster ions, but also the composition of precursor compounds and gas-phase impurities can be measured simultaneously. Using hexapole ion guides in the ioniAPi-TOF results in rather low fragmentation of weakly bonded cluster ions. Increasing the DC voltage of the second hexapole allows the study of collision induced fragmentation of weakly bonded cluster ions.

We will present first results of the positive ion composition obtained under very well controlled conditions during the CLOUD 12 campaign in fall 2017 at CERN, studying the influence of galactic cosmic rays on new particle formation. In addition, we will show results from an inter-comparison with the Tofwerk AG quadrupole APi-TOF of the University of Eastern Finland and discuss differences in the lower mass range <100 Th and similarities in the operational performance of the instruments in the mass range > 100 Th.

Acknowledgements: We thank the CLOUD collaboration (www.cern.ch/cloud) for the opportunity to test the new prototype instrument and for their support. This work is funded by the Austrian Science Fund, FWF (project no. P27295-N20), the Tiroler Wissenschaftsfonds (nanoTOF-ICE) and the University of Innsbruck promotion grant for young researchers.

6IM.7

Aerosol Chemistry Investigations by CHARON-PTR-ToF-MS. MARKUS MUELLER, Joris Leglise, Tobias Otto, Todd Rogers, Armin Wisthaler, *IONICON Analytik GmbH., Innsbruck, Austria*

Scientific progress in organic aerosol chemistry is still hampered by the lack of analytical methods that comprehensively and quantitatively characterize the organic composition of particulate matter in the atmosphere. Recently, the "Chemical Analysis of Aerosol Online" (CHARON) particle inlet has been introduced, enabling proton-transfer-reaction time-of-flight mass spectrometry (PTR-ToF-MS) instruments to characterize particulate-bound organics down to pg m^{-3} levels. Herein, we will demonstrate the potential of the CHARON-PTR-ToF-MS for aerosol chemistry and physics studies. Based on results from experiments on 36 pure compounds we will show how qualitative (elemental composition) and quantitative analyses (mass concentrations) can be corrected for biases caused by analyte ion fragmentation in the PTR-ToF-MS analyzer. We will further show how bulk elemental ratios (O:C, H:C) of urban aerosol and monoterpene-derived SOA compare with parallel TOF-AMS measurements and reported literature values. We will also compare the volatility of monoterpene-derived SOA on a molecular level as directly measured in thermodenuder experiments and predicted from the 2D-volatility basis set using the CHARON-PTR-ToF-MS-derived chemical composition. The implications for the aerosol chemistry of monoterpene-derived SOA will be discussed.

The development of CHARON was funded through the PIMMS ITN, which was supported by the European Commission's 7th Framework Programme under grant agreement number 287382. J.L. and T.O. received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement number 690958 (MARSU).

6IM.9

An Overview on Evaluation of the New Capture Vaporizer for Aerosol Mass Spectrometers (AMS). WEIWEI HU, Pedro Campuzano-Jost, Douglas Day, Benjamin A. Nault, Taehyun Park, Taehyoung Lee, Aki Pajunoja, Annele Virtanen, Philip Croteau, Manjula Canagaratna, John Jayne, Douglas Worsnop, Jose-Luis Jimenez, *CIRES, University of Colorado, Boulder*

The Aerosol Mass Spectrometer (AMS) and Aerosol Chemical Speciation Monitor (ACSM) are widely used for quantifying submicron aerosol mass concentration and composition. Using the standard vaporizer (SV) installed in almost all currently-operating instruments, a collection efficiency (CE) correction, varying with aerosol phase and chemical composition, is needed to account for particle bounce losses, which dominate the uncertainty on quantification of concentrations. To address this limitation, a new capture vaporizer (CV) was recently built and tested in various laboratory and field measurements. Here, we present an overview of results on CV quantification and spectrum characterization for laboratory-generated compounds and ambient aerosols, with comparisons results from co-sampled SV-AMS and other independent measurement. We found CV-AMS has an improved CE for less volatile compounds (e.g., pure $(NH_4)_2SO_4$ in the lab) and achieves CE~1 for ambient aerosols. However, the CV chemical detection properties show some differences from the SV due to the increased residence time of particles and vaporized molecules inside the CV, and different vaporizer materials. The effects of oxidation and heating of aerosols on quantification using both vaporizers is also examined. Artifact CO^+ ions (and to a lesser extent, H_2O^+), when sampling long chain reduced OA (e.g. squalene) in the CV, are observed, probably caused by chemical reactions between sampled OA and molybdenum oxides on the vaporizer surfaces (with the carbon derived from the incident OA). No evidence for such CO^+ enhancement is observed for highly oxidized species and ambient OA. The elemental composition and source apportionment (PMF) with the CV can be accurately determined after proper calibration. The size distribution broadening is significant for monodisperse particles, but its impact is limited in field studies since ambient distributions are typically quite broad. Consistent size distributions of ambient aerosols were measured with the SV and CV after calibration. Finally, we summarize all the relevant pros and cons when using the CV versus SV.

6MS.1

Facile Synthesis of Magnetic Metal-Organic Framework Nanocomposites by Spray-Assisted Synthesis. MASARU KUBO, Manabu Shimada, *Hiroshima University*

Metal-organic frameworks (MOFs), which are the novel porous crystalline materials constructed by coordination bonds of metal ions and organic linkers, serve as promising materials for many applications such as adsorption and separation, catalysis, chemical sensing, and solar cell; owing to their excellent porous characteristics. Recently, integration of other functional materials into MOF structure is of keen interest to express synergistic effect. Especially, the incorporation of magnetic Fe_3O_4 nanoparticles into MOFs enables to deliver MOF materials by external magnetic field. The magnetic manipulation can be utilized for applications such as drug delivery, catalysis, adsorption and detection. The combination of MOFs and Fe_3O_4 nanoparticles have been realized by direct synthesis into MOF pore or heterogeneous growth of MOF onto the surface of Fe_3O_4 nanoparticles. However both techniques are inevitable to generate MOFs not incorporating Fe3O4 nanoparticles.

Recently we developed a new MOF synthesis method called a spray-assisted synthesis.[1] In this method, an MOF precursor solution is sprayed and subsequently dried to enhance a self-assembly of metal ions and organic linkers; which enables to form MOF nanoparticulate powder within 10 ms continuously. Generally, one-droplet-to-one-particles conversion is considered to be the typical particle formation in a spray based material processing. We considered that addition of Fe_3O_4 nanoparticles into an MOF precursor solution enables to disperse Fe_3O_4 nanoparticles in all sprayed droplet and in all MOF particles.

Hence , in this presentation, we demonstrate the synthesis of Fe_3O_4/MOF nanocomposite and their dye adsorption properties.

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6MS.2

Dynamics of Carbon Nanotube Aerogel Formation. Christian Hoecker, Bhalerao Ajinkya, Nikolaos Kateris, Jean de La Verpilliere, Brian Graves, ADAM M BOIES, *University of Cambridge, University of Minnesota*

The underlying mechanisms behind the formation of gas-phase synthesized carbon nanotube (CNT) aerogels within a floating-catalyst chemical vapour deposition (FCCVD) reactor are still not well understood. The production of a macroscopic material from nano components, allows for the process to produce continuous CNT materials that are in great demand. The mass-produced self-assembled CNTs have superior thermal, electrical and mechanical properties making them valuable for many industrial applications.

While the material properties and applications of mass-produced CNT aerogels are well documented, the criteria required for gelation have not been discovered. Attempts have been made to describe CNT aerogel formation by relating the individual CNT growth to particle size distributions in the reactor. These, however, disregard fundamental features of 1-D material collisions, CNT restructuring and the dynamics within the FCCVD reactor.

In this presentation, we report on the dynamics of 1-D materials undergoing Brownian motion, collisions and re-orientation. By employing both molecular dynamic and Langevin dynamic modelling, we demonstrate that under typical conditions the time-scale for collision is much longer than the time-scale for re-orientation of the CNTs. Upon collision the CNTs re-orient to align with each other to form bundles (5-20 CNTs/bundle) due to Van der Waals forces. At a critical dimension, the CNT bundling ceases and long-range connections are maintained, thus allowing the formation of an aerogel.

Our work demonstrates the dynamics of both CNT collisions and bundling. Langevin dynamic results show that CNT collisions when accounting for both translation and rotation are similar to those found for non-dimensional aggregate collisions when only translation is accounted for. Molecular dynamics modelling demonstrates that re-orientation occurs at short timescales, but grows with CNT length and diameter. The methods for molecular dynamic modelling of re-orientation are discussed and approaches to extend the length of CNTs within a reasonable computational time are presented.

The resulting bundles and gelation theories are used to describe the aggregation in CNT aerosols which eventually leads to an aerogel formed of CNTs within synthesis reactors. These findings can then, for example, be related to the continuous gas phase process for the bulk production of CNTs, to identify the critical length and number concentration of CNTs required for gelation. Identifying the critical criteria for aerogelation of 1-D materials will potentially unlock the ability to produce novel self-assembled materials in high throughput reactors, unlocking the potential for industrial scale up.

6MS.3

Growth of Sub-5 nm Metal Nanoclusters in Polymer Melt Aerosol Droplets. Yong Yang, Pankaj Ghildiyal, MICHAEL ZACHARIAH, *University of Maryland, College Park*

Ultrasmall metal nanoparticles are inherently unstable because of their high specific surface area. This work investigates how growth and aggregation of these nanostructures can be circumvented by incorporating them into a polymer matrix in an on-the-fly growth process. We demonstrate the formation of sub- 5 nm particles of Ni, Co and Cu nanoparticles in polymer matrix using an aerosol single-drop reactor approach. The rapid thermal pulse given to the aerosol particles enables the formation of nuclei and growth, with subsequent rapid quenching to freeze in the structure. The role of temperature as well as precursor concentration of the resulting size and morphology are discussed. A characteristic time analysis and an analysis of the particle size distributions lead to the conclusion that growth is governed by nucleation and surface growth with little coagulation or Ostwald ripening. Finally, we note that this aerosol route is amenable to scale-up for large scale production of nanoclusters that can either be used as is within the polymer or released by solvent extraction, depending on application.

6MS.4

Single Step Synthesis of N/Ti3+ Co-Doped TiO2 Photocatalyst in a Flowing Microdroplet. LIANG-YI LIN, Shalinee Kavadiya, Yao Nie, Bedia Begum Karakocak, Pratim Biswas, *Washington University in St. Louis*

TiO2 has been widely investigated as a semiconductor photocatalyst in many areas like air/water purification, hydrogen energy, and conversion of carbon dioxide into fuels (e.g., CO and CH4). Nevertheless, the realization of TiO2 materials for practical uses has been impeded by its insufficient catalytic efficiency, which mainly originates from the fast recombination of photogenerated electron-hole pairs. Moreover, its wide band gap (~3.2 eV) makes it active only in the UV region, so it does not to utilize most of the solar spectrum. In this study, a visible-light-active nitrogen (N)/Ti3+ codoped TiO2 particle is developed for CO2 photoreduction. The N/Ti3+-TiO2 is directly synthesized in micrometer-sized droplets through a simple and continuous furnace aerosol process for the first time. Titanium nitrate and hydrazine monohydrate are used as precursors. The UV-Vis results revealed that the band gap of the aerosol-made N/Ti3+-TiO2 was drastically reduced to 1.53 eV, much lower than that of the pristine TiO2. And the photocatalytic activity tests showed that the N/Ti3+-TiO2 displayed an average CO production rate of 47.2 µmol g-1 h-1, which is about 8.9 times as high as that of commercial Degussa-P25 under UV-Vis-NIR light. The crystallinity, bandgap, and surface defect of the material were tailored by manipulating the furnace temperature and N2H4/Ti molar ratio, and detailed analyses on the physicochemical properties and the structure-photoactivity relationship of the obtained materials are systematically investigated. This study provides a new insight into the design of high-performance semiconductor materials for a wide range photocatalytic applications.

6MS.5

Aerosol-assisted Synthesis of a Stable Perovskite Absorber Layer for Application in Photovoltaics. SHALINEE KAVADIYA, Joseph Strzalka, Robin Wheelus, Pratim Biswas, *Washington University in St. Louis*

Recent advances have enabled aerosol generation techniques to synthesize and deposit materials for various applications. These techniques are simple, scalable, and operate at atmospheric pressure. Moreover, they can be operated continuously and allow precise control of material properties (size, morphology, crystal structure, composition), which are the challenges for some of the solution-based techniques. Perovskite ($CH_3NH_3PbI_3$) solar cells have received huge attention from the solar photovoltaic community in past few years because of their high efficiency and low-cost fabrication. However, their poor stability in ambient condition (mainly humidity) hinders their outdoor application. The presentation will discuss an aerosol-based technique, electrohydrodynamic atomization (i.e., electrospray), for fabrication of highly stable perovskite layer of perovskite solar cells under ambient humidity (30-50% relative humidity).

A two-step deposition method is used to form the perovskite layer, where PbI_2 is spin coated, and CH_3NH_3I (MAI) is electro-sprayed on the PbI_2 layer at room temperature. Both the precursors then react and form perovskite ($CH_3NH_3PbI_3$). The key feature of this methodology is lowering the reaction rate between the two precursors by gradually supplying MAI in solid nanoparticle phase onto the PbI_2 layer. The slow reaction leads to the formation of smooth and moisture-resistant perovskite film compared to the film fabricated by conventional solution-based techniques such as spin coating. The stability of the devices under the ambient condition is tested for 5.5 months. The cells fabricated using the electrospray retain 75% of the initial efficiency on average. The presentation will further discuss change in the structural properties of perovskite under heat treatment, and highly humid environment ($\geq$ 80% relative humidity) investigated using in situ Grazing Incidence Wide Angle X-ray Scattering (GIWAXS) at Synchrotron Facility, Advanced Photon Source at Argonne National Laboratory.

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6MS.6

Exploring the Impacts of Drying Dynamics on Final Particle/Granule Morphology Using a New Droplet Chain Instrument. JIM WALKER, Rachael E.H. Miles, Jonathan P. Reid, *University of Bristol*

The evaporative drying of droplets dispersed in a gas phase to form solid granules is a key process in a wide range of industrial applications, from spray drying to produce functional nano- and micro-particles, the delivery of pharmaceuticals for inhalation, spray painting, and food processing. For example, liquid milk, which has a short shelf-life, relatively high mass and requires refrigeration, is often spray dried to a powder prior to storage or transportation.

The structure and density adopted by a granule as the solvent evaporates can vary significantly depending on the dynamics of the drying process. For example, by varying the Peclet number (Pe), a measure of the relationship between the evaporation rate and diffusion rate of colloidal particles within the droplet, structures as diverse as crystals, encapsulated solids, hollow spheres and buckled/deformed/folded shapes can be formed. The desired granular structure and density varies depending on the application and an unexpected change in structure, such as buckling, can have unfavourable consequences for the efficacy of the product. The drying conditions which control granule morphology are still poorly understood.

In this work we use a new falling droplet chain instrument to resolve the rapid drying dynamics of individual droplets containing particle dispersions over their full evaporative lifetimes and compare with the resulting granule morphologies. We examine the conditions, such as initial droplet size, drying rate and the composition and concentration of the colloidal dispersion, required to form granules of different morphologies with particular attention paid to the conditions which result in granule buckling.

The instrument creates a continuous train of droplets, dispensed using a droplet-on-demand generator, which appears as a static chain when stroboscopically illuminated at the dispensing frequency [1]. The uniformity of the dispensed droplets and the reproducibility of the drying events means each droplet in the chain represents a subsequent snapshot in the lifetime of an individual droplet. The exceptional temporal resolution at which measurements can be made (10 ms) is calculated from the reciprocal of the dispensing frequency. High resolution imaging allow the drying dynamics to be resolved by measuring properties including the volume equivalent diameter (density independent), the aerodynamic diameter (density dependent) and optical diameter with < 1 um accuracies. The initial droplet diameter, typically 30 – 80 µm, can be controlled by the dispenser and the evaporation rate controlled with a temperature controlled gas flow. The final granule morphologies are examined using offline analysis tools such as scanning electron microscopy (SEM).

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6MS.7

Synthesis of Nanoscale Composite of Inorganic Elements And Aerosol Based Delivery for Improving Plant Nutrition.

RAMESH RALIYA, Pratim Biswas, *Washington University in St. Louis*

Nanomaterials are being investigated for addressing food – energy and water nexus. However, the majority of such published literature used either single or two type of nanoscale materials mixture. Naturally, plants uptake multiple elements altogether from soil – nutrient mixture, therefore, we designed our experiments to mimic nutrient mixture of highly required nutrients sources. In the present investigation, we synthesized using an aerosol process a nanoscale composite of five active nanoscale materials of nitrogen, phosphorous, potassium, zinc, iron which were loaded in the nano-porous silica particles. The mean geometric size of the nutrient loaded particles were in a range between 150 and 200 nm. The synthesized particles were characterized for the physicochemical properties and long term-stability using electron microscopy, X-Ray diffraction, dynamic light scattering and photo-correlation spectroscopy. The synthesized particles were applied on jalapeno pepper plants using an advanced aerosol delivery approach and studied through the life cycle. We observed significant improvement in plant growth, development, flowering, number of fruits and their nutritional contents. In summary, the carefully synthesized composite of active nanomaterial, aerosol-based foliar delivery to plant leaves and their systematic release may have potential not only to improve crop production but overall to address food-energy-water-environment nexus.

6MS.8

Polymer Coating of Inorganic Semiconductor Nanoparticles by Aerosol Approach. Masoom Shaban, Jalal Poostforooshan, ALFRED P. WEBER, *TU Clausthal*

Polymer coated inorganic semiconductor nanoparticles (ISNs) have attracted great attention due to enormous applications such as biomedical, catalysis, electronics, etc. Generally, the ISNs−polymer nanohybrids have been synthesized in the liquid phase methods which an appropriate solvent and surfactants are always required and they include several time-consuming steps. Moreover, in order to improve the compatibility between ISNs and monomers, suitable surface modification of inorganic nanoparticles is usually necessary.

To overcome the drawbacks of conventional wet methods, the work presented here describes a novel and facile approach to produce various ISNs−polymer core-shell including ZnO, TiO_2, and Fe_3O_4 nanoparticles by a surfactant-free aerosol-based synthesis *[1]*. In this regard, fresh spherical ZnO nanoparticles were initially generated by spark discharge followed by the sintering furnace in the gas phase. The size distributions of the spark generated ZnO nanoparticles sintered at different temperatures were measured using a scanning mobility particle sizer (SMPS).

The resulting ZnO nanoparticles exhibit excellent performance in the photocatalytic surface-initiated polymerization of butyl acrylate monomer in the continuous aerosol–photopolymerization, within the average aerosol residence time of 35 s in the photoreactor. This method is based on heterogeneous condensation of monomer vapor around the surface of gas-born ISNs, which is then polymerized ‘‘in flight’’ under UV light irradiation. In this one-pot synthesis, ISNs act not only as inorganic cores, but also at the same time are able to release charge carriers (electron-hole pairs) upon photoexcitation which drive the free radical polymerization near their surface. Therefore, no added initiator is required. To further investigate the basis and the mechanism of our experimental results, the optical properties of ZnO nanoparticles during the UV irradiation in the gas phase process was simulated by a three-dimensional finite difference time-domain (FDTD) method. Moreover, the coating efficiency was evaluated by aerosol photoemission and the results demonstrate that monomer and polymer coating efficiency are 99% and 80%, respectively.

Then, to verify the generality of this method toward coating different kinds of ISNs, rod-like ZnO, TiO_2 P25, and magnetic Fe_3O_4 nanoparticles were used as inorganic cores and photoinitiators. Interestingly, the thickness of polymer shell can be easily adjusted at the desired nanoscale by tuning the monomer vapor pressure. The molecular structure of the core-shell nanoparticles was characterized using ^1H NMR, FTIR, XRD and UV−vis spectroscopy. The polymer shell was also confirmed by TEM and XPS methods.

Finally, to investigate the potential applications of the nanohybrids in the fabrication of novel composites, the successful change in the surface hydrophobicity of ISNs after the encapsulation with the polymer shell was confirmed by their preference for an organic solvent.

[1] M. Shaban, J. Poostforooshan, and A. P. Weber, *J. Mater. Chem. A*, **2017**, 5, 18651–18663.

6MS.9

High Throughput Synthesis of Aerosolized Poly(3,4-ethylenedioxythiophene) (PEDOT) Nanoparticles for Water Dispersible Colloids. Lu Yang, Clayton Kacica, Shinjita Acharya, Yifan Diao, Luciano Santino, Hongmin Wang, Pratim Biswas, JULIO D'ARCY, *Washington University in St. Louis*

The conducting polymer poly(3,4-ethylenedioxythiophene) (PEDOT) is an organic electronic that serves as the active species in a plethora of applications for storing and harvesting energy as well as for sensing biological reactions. Moreover, this flexible soft material is characterized by high physical and chemical stability and a controllable and reversible doping mechanism that results in robust device performance. Current synthetic strategies for producing PEDOT employ a radical oxidative polymerization that is commonly carried out via solution oxidation synthesis, electrochemistry, or vapor phase deposition. Here we demonstrate a cutting edge route for making PEDOT using aerosolized aqueous droplets of the oxidant FeCl3 that react with vapors of the monomer 3,4-ethylenedioxythiophene inside a tube reactor. Our scalable and continuous high throughput approach results in spherical nanoparticles of PEDOT that are electrically conducting with a 300 ohm surface resistance; PEDOT nanoparticles are dispersible in water without the need of additives or surfactants. Colloids produced are stabilized by the polymer surface charge and solution processed to fabricate electrochemically active electrodes that store energy. Here we correlate polymerization kinetics and residence time to a polymer's crystal structure and its electrochemical activity in pseudocapacitors. Our work demonstrates high throughput processing of 500 nm diameter particles in gram quantities for delivering both high energy and power densities. We believe that this aerosol synthesis paves the way for a new route to producing this commercially important soft material and highlights the versatility of aerosol synthesis for producing the next generation of conducting polymer nanostructures.

6TT.1

Machine Learning to Predict the Global Distribution of Aerosol Mixing State Metrics. Michael Hughes, Jack Kodros, Jeffrey R. Pierce, Matthew West, NICOLE RIEMER, *University of Illinois at Urbana-Champaign*

Atmospheric aerosols are evolving mixtures of chemical species, and the term "mixing state" is often used to characterize this mixture. A population in which each particle is composed of one chemical species is called externally mixed, one where all particles are the same mixture of species is internally mixed, and real populations lie in between. In global climate models (GCMs) the aerosol mixing state is represented in a highly simplified manner. For example, modal models represent all aerosols within a given mode as internally mixed, while different modes are considered externally mixed. Failing to capture the true aerosol mixing state of ambient aerosols can introduce errors in the estimates of climate-relevant aerosol properties, such as the concentration of cloud condensation nuclei.

The goal for this study is to determine a global spatial distribution of aerosol mixing state with respect to hygroscopicity, as quantified by the mixing state metric χ. In this way, areas can be identified where the external or internal mixture assumption is more appropriate. Calculating χ requires detailed per-particle composition information, which is not possible to directly predict in GCMs. We therefore used the output of a large ensemble of particle-resolved box model simulations in conjunction with machine learning techniques to train a model of the mixing state metric χ. This lower-order model for χ uses as inputs only variables known to GCMs, enabling us to create a global map of χ based on GCM data. We found that χ varied between 20% and nearly 100%, and we quantified how this depended on particle size, location, and time of the year. This framework demonstrates how machine learning can be applied to bridge the gap between detailed process modeling and a large-scale climate model.

6TT.2

Simulation of Heterogeneous Oxidation of SO2 and NOx in the Presence of Gobi Desert Dust Particles under Urban Environments.

ZECHEN YU, Myoseon Jang, *University of Florida*

Large quantities of mineral dust particles are frequently ejected into the atmosphere through wind action. The surface of mineral dust particles can act as an import sink for atmospheric tracers (i.e., O_3, SO_2, NO_x and hydrocarbons) and photochemically enhance the production of oxygenated compounds. The photochemically oxidized hydrocarbons in the gas phase partition onto dust particles and involve in dust-phase heterogeneous reactions. These products modulate the characteristics of dust surfaces. In this study, we simulate the oxidation of SO_2 and NO_x in the presence of mineral dust under the ambient conditions using the Atmospheric Mineral Aerosol Reaction (AMAR) model. The model consists of explicit reaction mechanisms in three phases: gas phase, inorganic salted aqueous phase, and dust phase. Dust heterogeneous chemistry begins with a gas-particle partitioning process and is further processed *via* both autoxidation and photocatalytic oxidation by the dust phase semi-conducting matters. The simulation using the model is compared with UF-APHOR chamber data for the formation of nitrate and sulfate in the presence of Gobi Desert Dust particles and different hydrocarbons (i.e., 2-Methyl-2-butene, alpha-pinene, toluene, isoprene, gasoline and urbane mix hydrocarbons). In the exploratory experiment, the organic compounds formed from the photooxidation of 2-Methyl-2-butene in the presence of NO_x showed a negligible effect on dust-phase nitrate formation. However, oxidized compounds formed from the photooxidation of secondary organic aerosol precursor hydrocarbons (i.e., alpha-pinene) depleted dust phase nitrate that formed *via* the reaction of alkaline carbonates with nitric acid. The adsorbed ozone on dust surfaces can positively modulate the formation of sulfate and nitrate. Using the AMAR model that is integrated with the Carbon Bond mechanism (CB6), the influence of ozone on sulfate and nitrate formation in dust particles will also be simulated under the urban environments that contain various hydrocarbons and NO_x.

6TT.3

Photochemical Model Estimated Fire Impacts on Aerosol Evaluated with Field Studies and Routine Data Sources. KIRK BAKER, *United States Environmental Protection Agency*

Highly instrumented field studies provide a unique opportunity to evaluate multiple aspects of photochemical grid model representation of fire emissions, dispersion, and chemical evolution. Fuel information and burn area for a specific fire coupled with near-fire and downwind chemical measurements provides information needed to constrain model predicted fire plume transport and chemical evolution of important pollutants such as particulate matter (PM2.5) that have deleterious health effects. Most local to regional scale field campaigns to date have made relatively few transects through plumes from fires with well characterized fuel type and consumption. While more comprehensive field studies are being planned for 2018 and beyond (WE-CAN and FIREX), existing measurement data from multiple field campaigns including 2013 SEAC4RS, satellite data, and routine surface networks are used to assess how a regulatory modeling system captures fire impacts on local to regional scale PM2.5. A comparison of Community Multiscale Air Quality (CMAQ) model estimated speciated PM2.5 from specific fires with routine surface measurements at rural locations in proximity to the 2013 Rim fire, 2011 Wallow fire, and 2011 Flint Hills fires indicate PM2.5 organic carbon tends to be overpredicted at rural surface sites downwind from the 2011 Flint Hills prescribed fires while results were mixed at rural sites downwind of the 2013 Rim fire and 2011 Wallow fire. These results suggest differences in fuel characterization (e.g., emission factors, emissions speciation, burn period, etc.) between these areas may contribute to differences in model prediction. Remotely sensed AOD and aircraft transects made downwind of the 2013 Rim fire suggest the model does well at predicting local to regional scale transport and also the vertical extent of the plume. However, the model tends to underestimate regional downwind AOD compared with satellites and ground-based estimates during the Rim fire period.

6TT.4

Effects of Near-Source Coagulation of Biomass Burning Aerosols on Global Predictions of Aerosol Size Distributions and Implications for Aerosol Radiative Effects.

EMILY RAMNARINE, Jack Kodros, Jeffrey R. Pierce, *Colorado State University*

Motivation: Biomass burning is a significant global source of aerosol number and mass. Aerosols scatter and absorb solar radiation along with potentially acting as cloud condensation nuclei, affecting cloud albedo and lifetime. These climatic effects are known as the direct radiative effect (DRE) and the cloud-albedo aerosol indirect effect (AIE), respectively. These effects are influenced by the size distribution of the aerosol. Coagulation of particles is an important process in determining this size distribution. As coagulation occurs, the number of particles is diminished and the distribution is shifted to a larger mean diameter.

Sakamoto et al. (2016) found that the rate of growth by coagulation of a single fire plume can be approximated using the emissions rate of biomass burning aerosol mass, initial size distribution median diameter and modal width, plume mixing depth, and wind speed. This parameterization is physically intuitive as more concentrated emissions or emissions that are harder to dilute (due to larger emissions fluxes, larger fires, smaller wind speed, or smaller mixing depth) lead to the signatures of faster coagulation.

Methods: To explore the effects that coagulation has on global aerosol size distributions, we incorporated this parameterization into GEOS-Chem, a global model, with TwO Moment Aerosol Sectional (TOMAS) microphysics and fire emissions from the Fire INventory from NCAR (FINN). In the default configuration of GEOS-Chem-TOMAS, the fire emissions are given a fixed size distribution regardless of fire characteristics and meteorology. We adjust this emitted size distribution by aging it for one day using the above parameterization while keeping the mass of emissions constant. We use the rapid radiative transfer model for global climate models (RRTMG) on our GEOS-Chem-TOMAS aerosol output to study the effect that coagulation has on the DRE and AIE.

Sensitivities simulations: We test the sensitivity to two major uncertainties in our simulations. First, the initial size distribution of biomass burning emissions is important to the coagulation parameterization, but is not well known. To address this uncertainty, we have tested a range of initial median diameters and lognormal modal widths. Another uncertainty regarding the subgrid smoke coagulation parameterization is how much the smoke plumes overlap while coagulation is occurring. Plumes that do not overlap dilute more quickly than those that overlap and hence have less coagulation. We look at the two extreme cases: all plumes in each gridcell overlap instantly, creating one large plume, or they do not overlap at all.

Results: Our main results are as follows. (1) When there is more coagulation there is generally a smaller number of particles overall, but in some locations there is a high number of particles at small diameters due to a microphysical feedback creating more nucleation. (2) In regions/cases with more subgrid coagulation, there is lower sensitivity to uncertainty in the initial size distribution. (3) Regions and cases with more coagulation have fewer CCN-sized particles, which leads to a decrease in the magnitude of the AIE of biomass burning particles, though the effect remains negative in all cases. (4) DRE due to biomass burning is negative but is not found to be sensitive to our assumed coagulation scheme or initial size distribution because the size distribution changes do not greatly impact the mass extinction efficiencies in our cases.

Recommendation: In order to improve our estimates of biomass burning size distributions and radiative effects, we need (1) estimates of how plumes merge and overlap in different regions and (2) improved estimates of emitted size distributions in different regions in our simulations.

Sakamoto, K. M. et al., Atmos. Chem. Phys., 16, 7709-7724, doi:10.5194/acp-16-7709-2016, 2016.

6TT.5

Air Quality Impact of Distributed Combined Heat and Power Facilities. BO YANG, K. Max Zhang, *Cornell University*

Distributed generation (DG) has been more generally used to supply energy to the end users. Compared with centralized generation, DG has many advantages. Generating power on-site eliminates the cost, complexity and inefficiencies associated with transmission and distribution. However, since on-site DG facilities are close to the end users, the hydrocarbon fuelled DG emissions could be an important health issue.

The on-site air quality impacts of two different DG facilities on university campuses were investigated. One is a biomass fuelled combined heat and power (CHP) system equipped with an electrostatic precipitator (ESP). The other is a natural gas turbine CHP system with duct burners and a heat recovery steam generator (HRSG). For the biomass system, two rooftop sampling stations with $PM_{2.5}$ and CO_2 analyzers were established in such that one could capture the plume while the other one served as the background for comparison depending on the wind direction. Four sonic anemometers were deployed around the stack to quantify spatially and temporally resolved local wind patterns. For the natural gas turbine system, the in-stack emission tests were conducted in 2010 and 2015. $PM_{2.5}$, NO_x and other gas emissions were recorded. The emission data over time were analyzed by comparing these two sets of measurements.

A CFD-based model, Comprehensive Turbulent Aerosol Dynamics and Gas Chemistry (CTAG), was employed to analyze the measurement data and estimate the spatial variations of near-source pollutants. The primary $PM_{2.5}$ dispersion and chemical transformation of gaseous pollutants were simulate using the real terrain, local buildings, and meteorological data.

The simulation results demonstrated the near-ground “hotspots” would pose potential health risks to building occupants since ultrafine particles could penetrate indoors via infiltration, natural ventilation, and fresh air intakes on the rooftop of multiple buildings. Furthermore, spatial distributions of high ground level concentrations obtained by using CTAG were different from those by using a Gaussian-based parameterized model, AERMOD, largely due to that the CFD-based CTAG model can capture the building downwash effect much better than Gaussian-based models. Building downwash causes emissions entrainment inside wake zones next to buildings and lead to elevated local air quality impact, especially when the DG facilities have comparatively shorter stacks in an urban area. The implications on mitigating on-site air pollution and the suggestions on permitting DG facilities were discussed.

6TT.6

The Mixing State of Aerosol Particles in Asian Outflow Observed in the Spring of 2017. CUIZHI SUN, Kouji Adachi, Kentaro Misawa, Joe Hing Cho Cheung, Charles C.K. Chou, Nobuyuki Takegawa, *Tokyo Metropolitan University*

Anthropogenic emissions of aerosols and trace gases from East Asia have large influences on air quality and climate both on regional and global scales. The mixing state of black carbon (BC) aerosols, which is a key parameter for investigating the radiative impact of aerosols, has not been well understood because analytical methods for quantifying the mixing state of BC is limited. We have conducted an intensive measurement campaign in Taiwan in the spring of 2017, with the main focus being on the chemical composition and mixing state of aerosols in Asian outflow. The measurement was made at the Cape Fuguei (CAFE) station (25°N, 121°E) located on the northern tip of Taiwan from February 21 to March 14 in 2017. The laser induced incandescence-mass spectrometric analyzer (LII-MS) was used to measure the chemical composition of aerosol particles classified by the mixing state of BC. The combination of online LII-MS measurements and offline transmission electron microscope (TEM) analysis can provide useful insights into the variability in the mixing state of aerosols in Asian outflow. The other instruments include an Aerodyne mini aerosol mass spectrometer (mini-AMS), a particle-into-liquid sampler coupled with ion chromatography (PILS-IC), and filter sampling. A comparison of the LII-MS, mini-AMS, PILS-IC, and filter data demonstrates that sulfate, nitrate, and BC were quantified with reasonable accuracy.

Large enhancements in the mass concentration of PM2.5 aerosols were found during the measurement period. Backward trajectory analysis suggests that the enhancements were not due to local sources but to regional transport of air masses from the Asian continent. Sulfate was found to be the dominant chemical composition of fine mode aerosol particles. Nitrate was relatively minor in fine mode and abundant in coarse mode aerosols. The LII-MS data shows that the mass fraction of sulfate internally-mixed with BC was as high as 15% in highly polluted air masses. The variability in the mixing state of BC observed by the LII-MS was qualitatively consistent with that obtained from the TEM analysis. Factors affecting the variability and possible dependence of the LII-MS sensitivity to various types of mixing state (e.g., shell-core, attached) are discussed in detail.

6TT.7

Between Two Oceans: Auckland's Urban Aerosol. GUY COULSON, Gustavo Olivares, Sally Gray, Oliver Wilson, *National Inst of Water & Atmospheric Research, New Zealand*

Auckland, the largest city in New Zealand, is unique in being the largest city in the World to be almost completely surrounded by ocean and hence have no up or downwind sources of pollution. The city lies on a narrow isthmus between the Pacific Ocean and the Tasman Sea. Because of the lack of outside sources, average urban background concentrations of between 1000 and 4000 particles/cm3 are common away from major sources with very steep concentration gradients approaching sources such as roads (Pattinson et al., 2014). Consequently, Auckland's typical urban aerosol tends to be similar to other cities in character but with lower concentrations (Coulson et al 2015).

The Aerosol Tropospheric Chemistry in Urban Auckland (ATChU) experiment aimed to track the changes in aerosols and aerosol precursors as they move from open-ocean (clean background) across the city (polluted) and out into ocean again. Auckland has two prevailing wind directions WSW from the Tasman and ENE from the Pacific, so a transect along this line will almost always be in the prevailing wind direction. The experiment measured various aerosol parameters including composition, Black Carbon, particle number and size distributions along with gaseous pollutants simultaneously at three points across Urban Auckland, one on the upwind coastal urban edge, one in central Auckland and one on the downwind coastal urban edge for a period of approximately one month during March and April 2015.

Results from the west coast site have a similar character to the central Auckland site but with lower concentrations and a noticeable marine influence, whilst the east coast site has a more marine character with some urban influence. This presentation will examine results from the ATChU campaign with an emphasis on looking for the urban influence in a marine setting.

[1] Pattinson, W., I. Longley and S. Kingham, Atmospheric Environment Volume 94, Pages 782-792(2014).
[2] Guy Coulson, Gustavo Olivares and Nick Talbot. (2016) Aerosol Size Distributions in Auckland. Air Quality and Climate Change Volume 50 No.1. February 2016

Acknowledgements: Thanks to Melita Keywood and Paul Selleck at CSIRO for measurements of chemical composition. This work was funded by NIWA under the Strategic Science Investment Fund - Impacts of Atmospheric Pollution Programme.

6TT.8

The Effect of Vegetation on the Deposition and Dispersion of Ultrafine Particles Carrying Different Charges. MING-YENG LIN, Gabriel Katul, Andrey Khlystov, Chia-Ren Chu, *National Cheng Kung University*

Ultrafine particles (UFP) continue to receive increased attention due to their dual role in cloud microphysics and human health. Charged UFP can contribute a significant fraction of total UFP concentration, yet their deposition onto vegetation remains a subject of inquiry. Given the areal coverage of vegetation over land, vegetation is commonly assumed to be a large sink for UFP. Despite its broad significance, previous laboratory studies mainly focused on neutral UFP deposition onto canopies. Here, wind tunnel experiments are used to investigate the effect of vegetation on the deposition and dispersion of UFP carrying different charges.

To characterize the effect of vegetation on the deposition of UFP (size range 12.6 – 102 nm) carrying different charge, a small wind tunnel was first used. Juniper branches (*Juniperus chinesis*) covered the entire working section of this wind tunnel (i.e., the air flow is only through vegetation) and particle collection was determined from concentration differences across the vegetation section. Three different wind speeds were used (0.3, 0.6, and 0.9 m/s) in the experiments and their results were interpreted using single fiber theory. Results indicate that single fiber theory can be used to represent deposition of singly-charged UFP onto vegetation if both the image force and Brownian diffusion are simultaneously considered.

To investigate the effect of roadway vegetation on the dispersion of UFP carrying different charge, a boundary layer wind tunnel was used in this experiment. A line source simulating traffic emission was constructed and different row of trees (zero, one, and two rows) were used to explore the effect 'vegetation barriers' on UFP dispersion. A Tandem Differential Mobility Analyzer (TDMA) system was employed to examine the dispersion of UFP carrying different charges downwind of the roadway vegetation. Three different wind speeds (1, 2, and 3 m/s) were also tested. Preliminary results indicate that charged UFP number concentration decreases downwind of the vegetation as expected, the decay rate of charged UFP is faster than neutral UFP. The study results provide guidance for future climate and air quality models incorporating UFP.

6TT.9

Improved Estimation of Organic Aerosol Volatility Distributions by Combining Thermodenuder and Isothermal Dilution Measurements. KERRIGAN CAIN, Eleni Karnezi, Spyros Pandis, *Carnegie Mellon University*

Volatility is one of the most important physical properties of organic aerosol (OA), as it determines the partitioning of its components between the gas and particulate phases and eventually, their atmospheric fate. Most studies have estimated the OA volatility distribution using a thermodenuder (TD); however, the resulting distributions were quite uncertain. In this work, we test the hypothesis that the combination of TD and dilution measurements can better constrain OA volatility distributions over a wide range.

In this study, the method of Louvaris et al. (2017) combining TD and isothermal dilution measurements was refined using secondary organic aerosol (SOA) generated from the ozonolysis and reaction with OH radicals of several different precursors. SOA was produced in a smog chamber and sampled with a TD followed by a high-resolution time-of-flight aerosol mass spectrometer (AMS) and a scanning mobility particle sizer (SMPS). Parallel to the TD, a dilution chamber partially filled with clean air was used to isothermally dilute the SOA. The mass fraction remaining as a function of TD temperature and time in the dilution chamber was monitored by the AMS and SMPS. Improved wall loss corrections were used in order to better account for evaporation in the dilution chamber. The thermograms were then used with the algorithm of Karnezi et al. (2014) to estimate the volatility distributions, effective enthalpies of vaporization, and accommodation coefficients of the SOA tested. The results indicated that TD measurements alone overestimate the amount of semi-volatile SOA components. Furthermore, when the dilution measurements were added, the uncertainties of the semi-volatile components and enthalpy of vaporization were reduced.

The combination of TD and dilution measurements shows improvement over current techniques to estimate OA volatility distributions and can be implemented easily into volatility studies already using a TD. The application of this technique to ambient aerosol can provide insight into OA volatility and the results can be used to update chemical transport models accordingly.

References:

Karnezi, E., Riipinen, I., and Pandis, S. N.: Measuring the atmospheric organic aerosol volatility distribution: A theoretical analysis, Atmos. Meas. Tech., 7, 2953-2965, 2014.

Louvaris, E. E., Karnezi, E., Kostenidou, E., Kaltsonoudis, C., and Pandis, S. N.: Estimation of the volatility distribution of organic aerosol combining thermodenuder and isothermal dilution measurements, Atmos. Meas. Tech., 10, 3909-3918, 2017.

7AC.1

Hygroscopicity Dependent Upon Reaction Between Components in Internally Mixed Sodium Pyruvate and Ammonium Sulfate Aerosols. Hui Yang, PANG SHUFENG, Yunhong Zhang, *Beijing Institute of Technology*

In atmosphere, some compounds are mixed in a particle. The chemical reaction between components can lead to gas-particle repartition of volatile species, which has the important effect on SOA formation and climate. Herein, the reaction between sodium pyruvate and ammonium sulfate was monitored by using the attenuated total reflectance Fourier transform infrared (ATR-FTIR).

With decreasing RH, the feature bands of sodium pyruvate and ammonium sulfate decreased gradually, indicating a depletion of sodium pyruvate and ammonium sulfate. At 65.5 % RH, a sharp and narrow peak at 1132 cm−1 appeared, which is accompanied by the degration of the band at 1095 cm-1 into a weak shoulder, suggesting the formation of crystalline sodium sulfate. As the continuous decrease in RH, the 1132 cm-1 peak became stronger, indicating more crystal sodium sulfate. So it can be concluded that the reaction between sodium pyruvate and ammonium sulfate reduced to sodium sulfate and release of ammonia and pyruvic acid release.

When the RH take a cyclic change, water content decreased to ~50% or original droplets. In the second RH cycle, water content can restore. So the water content decrease should rise from the particulate reaction which ended after a RH cycle. Because of changeable compositions, the efflorescence RH on second dehumidifying was 67.1%, slightly higher than that of 64.2% on first dehydration.

7AC.2

Resolving the Factors Governing Particle Phase Photochemistry. BRYAN R. BZDEK, Lara Lalemi, *University of Bristol*

Whereas gas phase photochemistry and its role in producing new particles and determining gas phase composition are relatively well understood, aerosol phase photochemistry is understudied in part because of the complexity of the system. For example, nanofocussing of light into aerosol particles results in nonhomogeneous light distributions that are highly size dependent. Moreover, photochemistry at the solution-air (or particle-air) interface has been implicated in production of atmospherically significant volatile organic compounds that may even produce new atmospheric particles. Finally, aerosol particles can access supersaturated and highly viscous solute states, potentially changing the rates of photochemical reactions as well as the ability for the products to diffuse throughout the particle. The goal of this work is to resolve the factors that govern aerosol photochemistry (i.e. particle size, surface composition, and bulk properties) and compare them to bulk systems. These experiments will utilise holographic optical tweezers, where a laser beam is focussed through a microscope objective to produce one or several optical traps that will capture airborne picolitre volume droplets. Droplet size and refractive index can be precisely retrieved through collection of a Raman spectrum. Droplet surface and bulk properties are quantified through precise measurement of the coalescence dynamics of two optically trapped droplets.

The photolysis of nitrate will be used as a model system to probe photochemistry in aerosol particles. In a first set of experiments, the loss of the nitrate signal in the droplet Raman spectrum will be monitored as a function of exposure to UV light and particle size. A second set of experiments will examine how photolysis rates change as the droplet viscosity is increased by adding a known amount of sucrose to the droplet. A third set of experiments will resolve the significance of the aerosol-air interface to photochemistry. These experiments will involve incorporating a photoactive surfactant (e.g. nonanoic acid) into the droplet and monitoring changes to droplet properties as the surface coverage is changed. Together, these experiments will identify and quantify which factors are most significant to determining photochemical rates in aerosol droplets.

7AC.4

The Role of Solvent Environment on the Production of Imidazoles in Secondary Organic Aerosol Mimicking Solutions Containing Glyoxal and Ammonium Sulfate. ANDREW BERKE, Tara Bhat, Emma Gubbins, Hunter Myers, Amanda Nwankwo, *Smith College*

The reaction between glyoxal and ammonium sulfate represents an important model system with which to study the non-oxidative production of light absorbing compounds in secondary organic aerosols (SOAs). SOA particles have access to hundreds or thousands of airborne chemicals as they age, and each of these chemicals have the potential to affect particle growth, physical properties, and the production of light-absorbing compounds, such as imidazoles. These compounds can subsequently influence a particle's climatic and human health effects.

Our research seeks to understand the role the solvent environment, due to the addition of non-reactive chemicals, plays in SOA-forming bulk-phase reactions between glyoxal and ammonium sulfate. We use small, atmospherically relevant chemicals to perturb the solvent matrix and then measure the formation kinetics of light-absorbing compounds and solution viscosity of the resultant mixture. Results will be presented for a series of short-chain alcohols and other relevant organic molecules with different functional group moieties (including diols, ketones, esters, and nitriles) that show a relationship between solution viscosity and the production of imidazoles. Reasons for the observed behavior are also explored.

7AC.5

Investigating the Link between Molecular Mass, Volatility, and Optical Properties of Light-absorbing Organic Aerosols.

KHAIRALLAH ATWI, Zezhen Cheng, Rawad Saleh, *University of Georgia*

Organics produced from incomplete combustion span a wide range of light-absorption properties. We have directly investigated the relation between the light-absorption properties and molecular weight and volatility by conducting controlled combustion experiments using benzene as a model fuel. Combustion conditions were controlled by varying the flow rates of air and benzene and by controlling the temperature at which the combustion took place. At each combustion condition, the absorption coefficients (measured online using a photoacoustic spectrometer at 780, 532, and 420 nm) and the size distribution (measured using a scanning mobility particle sizer) were used to calculate the mass absorption cross section (MAC) and the absorption Ångström exponent (AAE). The particles were also collected on Quartz filters for offline analysis using laser desorption ionization time-of-flight mass-spectrometry (LDI-TOF-MS). The advantage of using LDI is that it can detect large molecules intact, allowing us to follow the formation of large organics from a several hundred to thousands of AMUs. Those measurements were also performed after heating the emissions in a thermodenuder operated at different temperatures to investigate the contribution of organics of different volatility to the total absorption cross section of the particles.

The light-absorption properties of the organic combustion particles generated spanned a wide spectrum, with MAC at 532 nm ranging from 0.4 to 2.4 m^2g^{-1} and AAE ranging from 9 to 3. The mass spectra produced using LDI-TOF-MS showed 24 AMU-spaced, regularly repeating peaks previously observed in the soot formation literature, with masses ranging between 200 and 2000 AMU. More importantly, there was a clear correlation of the molecular weight distribution of the organics with their light-absorption properties: the darker the samples (larger MAC and lower AAE), the more shifted were their mass spectra towards larger molecular sizes. Our experiments also show that as the particles were stripped of their more volatile components in the thermodenuder, their MAC increased and AAE decreased, indicating that the less volatile components are more absorptive. At a thermodenuder temperature of 400 C, the residual organics were extremely highly absorptive, with MAC and AAE of 3 m^2g^{-1} and 1.5, respectively. Furthermore, the mass spectra of the thermodenuded samples had a largely diminished signal in the low molecular weight region, indicating that they consist of larger compounds. These findings provide physical evidence of the relation between the molecular weight of the compounds and their volatility and optical properties, with volatility decreasing and light-absorption across all wavelengths increasing with increasing molecular weight.

7AC.6

Observations of Sulfate Aerosol Condensation in Flue Plumes from Coal-Fired Power Plants Equipped with WFGD.

JIANMIN CHEN, Xiang Ding, Di Wu, Xianmang Xu, Qing Li, *Fudan University*

More than half of the annual worldwide coal consumption is consumed in China, where about a half is used for electricity generation. Coal combustion is acknowledged to be one of the largest contributor to China’s haze pollution. Therefore, a new regulation for controlling air pollutant emissions from coal-fired power plants (CFPPs) has been executed in 2014. This policy has been called the standard of “Ultra Low Emission”. To meet the standard, all CFPPs are required to install flue gas desulphurization (FGD) and denitration systems. More than 90% of FGDs use the wet process of limestone-gypsum FGD technology, which is also the world’s most widely used FGD technology to remove SO2 and particulate matters (PMs). However, there is always a long “White Plume” emitted from industrial stacks, if it installed a wet FGD. The “White Plumes” have being attracted great public interest due to their possible negative effects on climate and health risks.

This study firstly reports characteristics of PMs in the “White Plumes” based on measurement at three CFPPs equipped with limestone-gypsum or seawater FGDs. Mass concentrations of water soluble ions (WSIs) in PM samples collected at wet FGD outlets were about 70-90% higher than that collected at the FGD inlets. Highest values were observed for PMs collected in the “White Plumes”. The relative percentage of sulfate ions (SO42-) in total WSIs were about 27%, 54%, and 64% in the three locations, respectively, while relative percentage for ammonia ions (NH4+) were about 11%, 16% and 16%, respectively. Droplets collected in the “White Plumes” showed acidity with a pH in the range of 2 ~ 4 and high WSI concentrations of about 3 ppb. The relative percentage of SO42- and NH4+ in total WSIs were about 63% and 18%, respectively. The increased values of SO42- and NH4+ in plumes are probably due to the condensation of SO2/SO3 and NH3 (slipped from denitration systems), since the temperature of flue gas in stacks (about 25 oC and 50 oC for seawater and limestone-gypsum FGDs, respectively) is generally higher than that of ambient air.

These condensable species, including H2O, SO2/SO3, NH3, and VOCs, can condense on existing PMs via heterogeneous nucleation. The results indicate that reported results in previous publications (obtained in stacks) commonly under-estimate the primary PMs emitted from CFPPs equipped with wet FGDs, especially SO42- and NH4+ concentrations. These experimental findings improve the basic understanding of potential climate and health effects of the “White Plumes”.

7AC.7

Daytime and Night-time Atmospheric Aging of Emissions from Combustion Related Sources by Electrospray Ionization Time-of-Flight Mass Spectrometry (EESI-TOF) in a Smog Chamber. AMELIE BERTRAND, Bin Yuan, Giulia Stefenelli, Yandong Tong, Lu Qi, Liwei Wang, Felipe Lopez-Hilfiker, Sepideh Esmaeilirad, Urs Baltensperger, Imad El Haddad, Jay G. Slowik, Andre S.H. Prévôt, *Paul Scherrer Institute*

Combustion processes are predominant sources of organic aerosol (OA). Several studies have reported their significant contribution to the ambient OA burden. In Europe, biomass burning often accounts for 30 – 50 % of the OA total concentration, while in Asia, coal combustion has been reported to account as up to 30 % of the OA total concentration. The contribution of these sources to the secondary fraction remain however largely uncertain. Due to the complex transformation of the emissions occurring over time in the atmosphere, source apportionment studies can fail to properly distinguish between the different origins of the secondary fraction.

To solve this hurdle, new instruments capable of providing a more extensive knowledge of the chemical composition of the OA at the molecular level and with a high time resolution are necessary. The Paul Scherrer Institute (PSI) has recently developed such an instrument: the extractive electrospray ionization time-of-flight mass spectrometer (EESI-TOF). The EESI-TOF enables real-time chemical analysis of atmospheric particles without thermal decomposition or ionization-induced fragmentation.

Here, we present results of the coupling of the EESI-TOF to a smog chamber to study the evolution during atmospheric aging of the chemical fingerprint of coal and biomass burning emissions generated with residential appliances. Experiments were conducted in the 7m3 atmospheric chamber (Teflon, 20 °C) of PSI. Emissions were oxidized during 4 - 5 hours under a variety of conditions (NO3 and OH chemistry) to simulate atmospheric aging both during the day and at night. A High Resolution – Time of Flight – Aerosol Mass Spectrometer (HR-TOF-AMS) and an Aethalometer AE33 were installed alongside EESI to provide real-time analysis of the bulk chemical composition of the particulate phase, including the non-refractory material and the black carbon. A Proton Transfer Reaction – Time of Flight – Mass Spectrometer (PTR-TOF-MS) was installed to monitor the volatile organic compounds.

We look into the modification of the chemical fingerprint during aging. With EESI we highlight the differences between fresh and aged, OH, and NO3 chemistry profiles, and compare with what is known of HR-TOF-AMS studies. We show time series of specific ions susceptible to serve as tracers for fresh biomass burning and coal combustion emissions, and secondary fraction. And finally we further investigate the evolution of certain of these compounds in the chamber in lights of what is known regarding their volatility and partitioning.

7AC.8

Understanding the Selective Transfer of Carbohydrates from the Ocean to Sea Spray Aerosol. ELIAS HASENECZ, Hansol Lee, Alexei Tivanski, Elizabeth Stone, *University of Iowa*

The ocean is a globally important source of atmospheric aerosols whose composition and properties are both climate relevant and under-examined. These properties, such as radiative forcing and cloud condensation nuclei activity, are influenced by the diversity of chemicals found in ocean derived aerosol. Surface active species are enriched at the ocean surface in the sea surface microlayer (SSML) and are selectively transferred to sea spray aerosol (SSA) via bubble bursting. Among organic matter enriched in SSA are carbohydrates, or saccharides, that primarily originate from biological sources and can comprise a significant portion of SSA organic mass. The selective transfer of a chemical species is facilitated by their properties and surroundings—for example, carboxylic acids are selectively transferred due to increasing surface activity, which is illuminated by decreases in the surface tension of the water interface. Determining the physicochemical processes that drive selective transfer of saccharides will ultimately improve our understanding of SSA composition and resultant globally relevant properties.

In this study, SSAs were produced with granular glass frit bubblers to determine how increasing the number of saccharide monomer units affects their transfer from bulk seawater to SSA. Sub-surface (bulk), SSML and SSA samples were collected using a 5 stage cascade impactor and analyzed for saccharides and ions via high performance ion exchange chromatography with pulsed amperometry and conductivity detection, respectively. Enrichment factors (EF) were calculated by dividing the saccharide-to-sodium ratio in the SSML or SSA by this ratio in bulk solution. To correlate our chemical speciation measurements to changes in physicochemical properties, solution surface tension was also measured using a force tensiometer. Saccharide monomers through hexamers showed no enrichment (EF = 1), which is consistent with no change in surface tension (73.5 ± 0.3 mN/m) and confirms these species are neither surface active nor enriched in the SSML or SSA. However, alginate, an acidic polysaccharide prevalent in seaweed, shows small enrichment (1.6 ± 0.2) in the smallest aerosol size fraction (Nevertheless, the small polysaccharide enrichment shown here is one to five orders of magnitude smaller than studies containing natural seawater and/or microbes, suggesting surface activity alone is not the main driving force for saccharide transfer. For future studies, microgels that are ubiquitous in the ocean, saccharide-rich, positively buoyant and enriched in SSA, will be studied for their capability to selectively transfer saccharides to SSA.

7AC.9

Environmental Factors Affecting Humic-like Substance Production in Photoreactions of Polycyclic Aromatic Hydrocarbons. JOHN HAYNES, Keith Miller, Brian Majestic, *University of Denver*

Humic-like substances (HULIS) are a class of light absorbing compounds and are present in the atmosphere as a collective of organic species, each containing significant aromatic and carboxylic acid character. They are found to be a major component of brown carbon and are connected with radiative forcing in the atmosphere. Aerosolized HULIS are consistently correlated with reactive oxygen species and soluble metals, and as such, they are implicated with respiratory problems, oxidative stress, and the production of phytoplankton in marine systems. Polycyclic aromatic hydrocarbons (PAH) and HULIS are commonly observed in particles sourced from pyrogenic processes, e.g. biomass burning and vehicle exhaust. PAH are produced by the inefficient burning of organic fuels and display extended lifetimes in the atmosphere. These aromatics are toxic to human health and many structures are considered highly carcinogenic. PAH have many atmospheric reaction pathways - one recently discovered endpoint is the formation of HULIS.

This bench study evaluates the impact of environmental changes on HULIS production by oxidation of suspensions of PAH with exposure to sunlight using several different matrix environments. The long range transport of PAH lend themselves to extended exposures to sunlight and reactive environments potentially producing branched and oxidized PAH products (oxPAH) which then act as intermediates for more complex structures, e.g. HULIS. This extended reactive exposure may be affected by changing cloud water environments, including buffer systems, dust entrainment, and soluble metals. Environmental PAH and HULIS are correlated with reactive oxygen species in cloud water and aerosolized particles. Atmospheric aromatics may incorporate ultraviolet radiation with redox reactions of buffered systems or bioavailable metals as photo-Fenton catalysts in an electron transfer interaction with elemental oxygen or water molecules to produce radicals, such as superoxide or hydroxyl radicals. These oxyradicals are highly reactive agents and may initiate several oxidizing pathways, resulting in the further production of HULIS via oxPAH. The introduction of environmental deviations may enhance or inhibit this production by favoring specific or new reaction pathways.

Reaction conditions use simulated sunlight introduced to varying PAH reagent and matrix composition, oxidizing agents, and temperature over 16 hours. Analysis of bulk products are performed using UV-vis, HPLC, and GCMS - used to define the spectroscopic properties and structure of these products. Solid phase extractions of HULIS material are analyzed by GCMS and ATR-FTIR. Initial reaction data include significant differences between dissolved and saturated PAH solutions, as well as changes in the production of oxPAH between soluble ferrous and ferric ion interactions with PAH. Comparison between systems are based on UV-vis analysis and the growth of new HPLC peaks during and following light exposure periods, which monitor the character and production of several new species. Continuous decays within the UV-vis chromatographic spectra and arrays of several products are observed for samples with soil and with dissolved ferric ions and are emblematic of HULIS materials. Comparing these products with strong differences in product data for reactions using dissolved PAH or spikes with ferrous ion are observed and are of particular interest. Evaluating the formation of products from dissolved and suspended PAH solutions with photo-reactions conducted with soluble metals, cloud buffer, and suspended soil allows for the determination of specific reaction mechanisms. A higher understanding of the creation of HULIS in atmospheric conditions will greatly aid in predictive models for air quality and human health downwind of pollution sources.

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7AC.10

Effects of Criegee Intermediate Scavenger on Secondary Organic Aerosol Formation during α-pinene Ozonolysis. KEI SATO, Shinichi Enami, Sathiyamurthi Ramasamy, Satoshi Inomata, Takashi Imamura, *National Institute for Environmental Studies, Japan*

Criegee intermediates (CI) might contribute to formation of low-volatility organic compounds such as dimers in the atmosphere. We used a laboratory environmental chamber to investigate the effects of CI scavengers on secondary organic aerosol (SOA) formation from α-pinene ozonolysis in the presence of OH radical scavenger. We used formic acid and heptanoic acid as the CI scavengers, and used carbon monoxide as the OH radical scavenger. Experiments were conducted under dry conditions (RH < 0.1%). Gaseous compounds were measured by FT-IR, and the chemical composition of SOA was measured by AMS. The SOA mass concentrations measured after the consumption of 0.1-ppm α-pinene in the experiments with heptanoic acid (262–275 μg m-3) were higher than those measured with formic acid (189–196 μg m-3) and without a CI scavenger (202–216 μg m-3). The O:C ratios measured for SOA in experiments with heptanoic acid (0.27–0.29) were lower than those measured with formic acid (0.31–0.36) and without CI scavenger (0.30–0.35). We also studied the addition effect of ammonium sulfate seed particles. Similar results were obtained in the presence of seed particles, but the SOA concentrations measured with seed particles are slightly higher than those measured without seed particles. The CIs formed from α-pinene ozonolysis react not only with α-pinene oxidation products but also heptanoic acid. The reactions of the CIs with heptanoic acid would result in formation of the SOA with O:C ratios lower than those formed during α-pinene ozonolysis.

7AC.11

The Predicted Impact of Organic Coatings on Isoprene-Derived Secondary Organic Aerosol Formation. WILLIAM VIZUETE, Mutian Ma, Yue Zhang, Sri Hapsari Budisulistiorini, Havala Pye, Jason Surratt, Yuzhi Chen, Ryan Schmedding, Sarah Farrell, *University of North Carolina at Chapel Hill*

Fine particulate matter (PM2.5) is known to have an adverse impact on public health and is an important climate forcer. Secondary organic aerosol (SOA) contributes to PM2.5 and the multiphase reactions between gas- and particle-phase constituents is an important source. Aerosol-phase state is thought to influence the reactive uptake of gas-phase precursors to aerosol particles by altering diffusion rates within particles. Current air quality models (AQM), however, do not include this feature. This work examines the predicted impact of organic coatings on the formation of SOA from the acid-catalyzed multiphase reactions of isoprene epoxydiols (IEPOX). New experimental studies have provided a systematic quantification of the reactive uptake coefficient (γ) of trans-β-isoprene epoxydiol (trans-β-IEPOX), the predominant IEPOX isomer, onto acidic sulfate particles with varying organic coatings. In some experiments the uptake coefficient was reduced by half of the original value when coatings were present. This new experimental data, and published kinetic rates, now allow for examination of constrains on critical parameters needed to simulate coating effects on reactive uptake. This work developed a 0-dimensional box model that incorporated the latest kinetic data that accounts for coating influences. Meteorological inputs and gas phase concentration data were provided from field measurements at the Look Rock, Tennessee (LRK) ground site during the 2013 Southern Oxidant and Aerosol Study (SOAS). The LRK site also provided particle-phase chemical data of IEPOX-derived organosulfates and 2-methyltetrols that was used for model performance evaluations.

Including a coating influence in the reactive uptake algorithm reduced predicted IEPOX-derived SOA on average by 31%. One critical parameter in the model algorithm was the inorganic Henry's Law coefficient (H), with a range of reported values from 2.7 6 M/atm to 4.0 8 M/atm. Sensitivity simulations from this work found that H had the greatest impact on predictions when a 10-fold increase led to 8-fold increase in SOA concentrations. The organic diffusion coefficient (Dorg) and organic Henry's Law coefficient (Horg) were also found to be a critical parameter. For these simulations, the reported 0.3 M/atm was used for Horg. In the literature Dorg has been derived as a function of relative humidity (RH) either from experimental measurements of IEPOX uptake on -pinene coated sulfate aerosols, or estimates from viscosity data of -pinene SOA. In these model runs when the Dorg is , IEPOX uptake was completely inhibited and when Dorg reached organic coatings had no effect. Using the LRK filter data, and published range of parameter values, a simulation was completed that produced the best model performance where the empirically derived Dorg from -pinene coated aerosols was used with a H of 8.0 7 M/atm and Horg of 0.3 M/atm. This simulation increased SOA concentrations improving the normalized mean bias to -24.7%.

These results suggest that the organic coating layer could have significant impact on the IEPOX-derived SOA formation and should be considered in AQMs. This work relied on organic diffusion coefficients derived from our previous -pinene SOA experiments, and thus, only represents one possible type of organic coatings in the atmosphere. Other organic coatings, such as those derived from anthropogenic and other biogenic sources (including isoprene itself) could have a different impact on the acid-catalyzed reactive uptake of IEPOX. Furthermore, part of the Dorg used in this work were derived with flow tube experiment data occurring only under RH conditions between 15-50% while the Dorg for higher RH are based on viscosity data and experimental extrapolation. Further experimental studies are needed to constrain these parameters in >50% RH environments.

7AC.12

Impact of Ammonium Nitrate Aerosol Formation on Ozone Production in Urban and Rural New York State. MATTHEW NINNEMAN, Sarah Lu, Pius Lee, Jeffery McQueen, James Schwab, *University at Albany, SUNY*

The nighttime deposition of ammonium nitrate aerosol (NH_4NO_3) onto surfaces is an important oxides of nitrogen (NO_x) removal pathway, which affects next-day photochemical ozone (O_3) production. Prior studies have mainly examined this phenomenon in either urban or rural environments. However, these studies have not compared the impact of NH_4NO_3 formation on O_3 production in urban versus rural locations. To address this research gap, this study used continuous NH_4NO_3, ammonia (NH_3), nitric acid (HNO_3), NO_x, and O_3 measurements taken in one urban location and one rural location in New York State (NYS) beginning in mid-2016. In addition, photochemical ozone production rates (P_{O3}) and concentrations of dinitrogen pentoxide (N_2O_5), water vapor (H_2O), nitrous acid (HONO) and gas-phase nitrate (NO_3) are determined for both sites using an air quality model. The urban and rural locations of interest were Queens College (QC) in Flushing, New York (NY), and Pinnacle State Park (PSP) in Addison, NY, respectively. The effect of NH_4NO_3 formation and deposition on next-day photochemical O_3 production differs at QC and PSP. This may be due in part to (1) differences in modeled N_2O_5 and NO_3 concentrations and measured NH_3, HNO_3, and NO_x concentrations, (2) differences in NO_x-sensitive versus NO_x-saturated environments, and (3) differences in the extent of poorly characterized NO_x sources from surface-enhanced re-noxification, all of which are explored in this study.

7AC.13

Mixing State of Oxalic Acid Containing Particles in the Rural Area of Pearl River Delta, China. CHUNLEI CHENG, Mei Li, Chak K. Chan, Haijie Tong, Zhen Zhou, *Jinan University*

The formation of oxalic acid and its mixing state in atmospheric particulate matter (PM) were studied using a single particle aerosol mass spectrometer (SPAMS) in the summer and winter of 2014 in Heshan, a supersite in the rural area of the Pearl River Delta (PRD) region in China. Oxalic acid-containing particles accounted for 2.5% and 2.7% in total detected ambient particles in summer and winter, respectively. Oxalic acid was measured in particles classified as elemental carbon (EC), organic carbon (OC), elemental and organic carbon (ECOC), biomass burning (BB), heavy metal (HM), secondary (Sec), sodium-potassium (NaK) and dust. Oxalic acid was found predominantly mixing with sulfate and nitrate during the whole sampling period, likely due to aqueous phase reactions. In summer, oxalic acid-containing particle number and ozone concentration followed a very similar trend, which may reflect the significant contribution of photochemical reactions to oxalic acid formation. The HM type particles were the most abundant oxalic acid particles in summer and the diurnal variations of peak area of iron and oxalic acid show opposite trends, which suggests a possible loss of oxalic acid through the photolysis of iron oxalato complexes during the strong photochemical activity period. In wintertime, carbonaceous type particles contained a substantial amount of oxalic acid as well as abundant carbon clusters and biomass burning markers. The general existence of nitric acid in oxalic acid-containing particles indicates an acidic environment during the formation process of oxalic acid. The peak areas of nitrate, sulfate and oxalic had similar temporal change in the carbonaceous type oxalic acid particles, and the organosulfate-containing oxalic acid particles well correlated with total oxalic acid particles during the episode, which suggests the formation of oxalic acid is closely associated with the oxidation of organic precursors in aqueous phase.

7AC.14

Fast Heterogeneous N2O5 Uptake and ClNO2 Production in Summer in Urban Beijing, China. WEI ZHOU, Jian Zhao, Bin Ouyang, Asan Bacak, Conghui Xie, Qingqing Wang, Junfeng Wang, Yuying Wang, Wei Du, Weiqi Xu, Archit Mehra, Stephen Worrall, Xinlei Ge, Penglin Ye, James Lee, Hugh Coe, Roderic Jones, Pingqing Fu, Zifa Wang, Douglas Worsnop, Yele Sun, *Institute of Atmospheric Physics*

The heterogeneous hydrolysis of dinitrogen pentoxide (N_2O_5) has a significant impact on nocturnal particulate nitrate formation and photochemistry on the secondary day through the photolysis of nitryl chloride ($ClNO_2$), yet their roles and processes in the highly polluted areas remain less understood. Here we present the measurements of gas-phase N_2O_5 and $ClNO_2$ by a high-resolution time-of-flight chemical ionization mass spectrometer during the Air Pollution and Human Health (APHH) campaign to investigate the nocturnal chemistry in summer in urban Beijing, China. N_2O_5 and $ClNO_2$ show large day-to-day variations that are closely related to their precursors (i.e., O_3 and NO_x). High reactivity of N_2O_5 with $\tau(N_2O_5)^{-1}$ ranging from 0.20×10^{-2} to 1.46×10^{-2} s^{-1} suggests active nocturnal chemistry and a large nocturnal nitrate formation potential via N_2O_5 heterogeneous uptake. We also observed high $ClNO_2/N_2O_5$ ratios, likely due to the correspondingly high $ClNO_2$ production rate under sufficient chloride in Beijing. The N_2O_5 uptake coefficients estimated from the product formation rates of $ClNO_2$ and particulate nitrate are in the range of 0.017-0.190, corresponding to the direct N_2O_5 loss rates of 0.00044-0.0034 s^{-1}. Further analysis indicate that the fast N_2O_5 loss in the nocturnal boundary layer in urban Beijing is mainly attributed to the indirect NO_3 loss pathway, for example, through the reactions with volatile organic compounds and NO, while the contribution of heterogeneous uptake of N_2O_5 is small (7-33%). We also observed high $ClNO_2$ yields ranging from 0.10 to 0.35 which might have important implications for air quality by affecting the nitrate and ozone formation.

7AC.15

Multivariate Statistical Analysis Methods as a Tool to Study Complex Mass Spectrometry Data Sets. SINI ISOKÄÄNTÄ, Eetu Kari, Angela Buchholz, Annele Virtanen, Santtu Mikkonen, *University of Eastern Finland*

Mass spectrometer measurements produce complex data with a large number of variables. In this work, we used different statistical dimension reduction techniques to compress the information from the data to a small number of factors, which can be further interpreted. Different variations of Positive Matrix Factorization (PMF), Exploratory Factor Analysis (EFA) and Principal Component Analysis (PCA) were applied to multivariate car exhaust emission data measured by proton-transfer-reaction time-of-flight mass spectrometry (PTR-ToF-MS). In the experiments, the diluted gasoline car exhaust was fed into an environmental chamber, and it was further photo-oxidized to clarify the possible reactions of gasoline car exhaust with OH-radicals in the atmosphere.

This work showed that different statistical methods produced similar results, but EFA created factors with the most plausible physical interpretation for the experiments. EFA separated PTR-ToF-MS measured car exhaust data into four different factors: Feeding factor, secondary organic aerosol (SOA) precursor factor, reaction side product factor, and reaction product factor.

The benefit of EFA and PCA compared to PMF is that these methods scale the variables and only the relative changes in concentrations are taken into account. Generally, this allows these methods to discover very small changes in the time series of the variables even if the concentrations are low. The advantage of PMF that PMF calculates the results in data units whereas EFA/PMF results have arbitrary units. In our work, however, we calculated the EFA/PCA factors also in the data units by multiplying the original data with the loading values (i.e. contribution of a variable to a factor) acquired from EFA/PCA. This allowed us to compare the factor time series from different methods reliably. This work demonstrated that all statistical methods tested offered valuable tools for complex data set analysis. Particularly, EFA was useful in this specific case because it identified the most interpretable factors from the experiments.

7AC.16

Molecular Diffusion Limitations Coupled with Aerosol Aging Initiated by Iron Citrate Photochemistry. PABLO CORRAL ARROYO, Peter Aaron Alpert, Jing Dou, Beiping Luo, Ulrich Krieger, Markus Ammann, *Paul Scherrer Institut*

Physical and chemical transformations that change the properties of atmospheric particles are known as aerosol aging. Understanding of these is essential to evaluate their impact on climate, air quality and health. Photochemistry may start aging processes by the presence of chromophores in aerosol particles that act as photocatalysts inducing oxidation of non-absorbing molecules [1]. Iron (Fe(III)) carboxylate complexes absorb light below about 500 nm followed by ligand to metal charge transfer (LMCT), the reduction of iron to Fe(II) and oxidation of the carboxylate ligands, a process that is recognized as an important sink of organic acids in the troposphere [2]. We investigate the feedbacks between these photocatalytic processes and molecular diffusion within aerosol particles. To achieve this scope, iron oxidation within mixed iron citrate and citric acid (1:1 molar ratio) particles is spatially mapped before and after irradiation with UV light (370 nm) using scanning transmission X-ray microscopy with near edge X-ray absorption fine structure spectroscopy (STXM/NEXAFS). This yields 2D-projected Fe(II) and Fe(III) fractions with 35x35 nm resolution. We observed gradients in the composition of single aerosol particles which indicates oxygen diffusion limitation. Additionally, we measure the release of HO_2 radicals and volatile organic compounds (VOCs) to the gas phase when films loaded with iron citrate and citric acid in Coated Wall Flow Tube (CWFT) are irradiated with light. The nonvolatile compounds produced after irradiation are analyzed by HPLC-MS. Finally, we present a numerical photochemical and molecular diffusion model to explain our results. We have found that particles can be devoid of oxygen due to reacto-diffusive limitation and thus, maintain reduced particle cores despite being surrounded to the oxygen rich atmosphere. This is counter to a typical concept that oxygen saturates atmospheric aerosol.

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7AC.17

A Combination of a Cavity Ring Down Spectrometer and an Electrodynamic Quadrupole to Retrieve Physical and Optical Constants from Single Trapped Particles. ANTONIO VALENZUELA, Jonathan P. Reid, Allen E. Haddrell, Bryan R. Bzdek, Rose Willoughby, Andrew J. Orr-Ewing, *University of Bristol*

The rapid changes in climate observed during recent decades have important social and economic impacts on both global and regional scales that have brought climate change into the spotlight worldwide. According to the Fifth Assessment Report (AR5) of the last Intergovernmental Panel on Climate Change (IPCC) in 2013, atmospheric aerosol produces a net cooling effect of the Earth's climate. However, an accurate estimate of this cooling is extremely difficult because of the large uncertainty on the estimation of the aerosol radiative forcing (RF), where the largest uncertainty in RF is due to uncertainties in understanding aerosol properties. Reduction of these uncertainties requires improved methods of laboratory determination of the optical properties of aerosol particles and their change with ambient relative humidity. Cavity ring-down spectroscopy (CRDS) has been proven to be a sensitive tool for measuring the absolute extinction cross-sections for single aerosol particles with high precision by combining optical confinement and levitation of a particle with CRDS (1). Studies on single particles, confined within optical or electrodynamic traps, provide precise measurements of aerosol refractive indices, hygroscopic growth, evaporation of semivolatile components, and other properties of importance for their atmospheric behavior. However, overall, these studies have been focused on characterizing optical and physical properties of non-absorbing aerosols. In this sense, we have designed and built an Electrodynamic Quadrupole (EQ) trap to confine and levitate a wide range of different single aerosol particles even absorbing particles. We present a new experimental approach which uses a combination of CRDS and an EQ trap which will allow the measurements of absolute light extinction cross-sections and optical constants and their dependence on environmental conditions over an extended time frame for single aerosol particles. We expect to extend previous analysis centered on non-absorbing aerosols to the more challenging case of absorbing aerosols allowing direct determination of the change in physical and optical properties of micrometer-sized aerosol particles over time. We will demonstrate that such a single particle technique leads to a significant reduction in the uncertainty in the complex refractive index, reducing, for example, the uncertainty in the real part to ±0.3 % and retrieving a more precise imaginary part for absorbing aerosols. We will report retrievals of optical properties of aerosol spanning from simple mixtures of organic components through to samples of laboratory surrogates of secondary organic aerosol.

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7AC.18

Radiative Absorption by Light Absorbing Carbon: Uncertainty, Seasonal and Spatial Variation in a Typical Polluted City in Yangtze River Delta. DONG CHEN, Yu Zhao, Ritao Lyu, Jie Zhang, *Nanjing University*

One of the major challenges in understanding radiative forcing by aerosols is to accurately monitor and assess the light absorbing components and their contributions to climate forcing in the present-day atmosphere. In this study, the optical properties of light absorbing carbon (LAC) in aerosols, including its temporal and spatial variations were studied at suburban (NJU), urban (PAES) and industrial (NUIST) sites in Nanjing, a typical polluted city in Yangtze River Delta (YRD). It was found that the application of constant values for multiple scattering factor could not well represent the actual absorption characteristics of aerosols in Nanjing. The relative deviation between calculated and measured absorption coefficients of BC was up to 56 ± 34%. An improved method that applied local multiple scattering correction factors could reduce the uncertainty to less than 5%. Distinct seasonal variation exhibited in the mass absorption efficiency ($MAE_{BrC,365}$) of brown carbon (BrC) at NJU. BrC from secondary sources had a stronger absorption ability than that from primary emissions such as diesel vehicles in winter. $MAE_{BrC,365}$ in autumn when the SOA precursors were dominated by anthropogenic volatile organic compounds (VOCs) was 1.9 times higher than that in summer when biogenic VOCs were the main secondary organic aerosol (SOA) precursors. At industrial site, BrC was mainly formed by aged secondary organic carbon (SOC) and had a stronger light absorbing ability than that at other two sites. The results of simultaneous observation at NJU and PAES indicated that formation of fresh BrC enhanced the optical absorption of BC but reduced that of BrC. This study indicates the necessity of measurement of local multiple scattering factor for evaluation of BC absorption and implies possible ways to alleviate the light absorption effect of LAC.

7AC.19

Chemical Composition Changes during Secondary Organic Aerosol Particle Evaporation. ANGELA BUCHHOLZ, Arttu Ylisirniö, Claudia Mohr, Celia Faiola, Eetu Kari, Andrew Lambe, Zijun Li, Aki Pajunoja, Sergey Nizkorodov, Siegfried Schobesberger, Douglas Worsnop, Taina Yli-Juuti, Annele Virtanen, *University of Eastern Finland*

The partitioning of compounds between gas and particle phase can be described with the Volatility Basis Set (VBS), which group them by their saturation vapor pressure. In previous studies, slower evaporation than expected from VBS distributions was observed for α-pinene particles at dry conditions. This could be caused by physical limitations or by chemical processes in the particle phase. It is therefore important to study the changes of the chemical composition of particles during evaporation to gain insights into the processes governing particle evaporation.

We investigated Secondary Organic Aerosol (SOA) from photooxidation of a-pinene with three different O:C ratios (0.55, 0.70, and 0.95). Monodisperse particles were fed into a Residence Time Chamber (RTC), which was at 0%, 40%, or 80% RH, to study evaporation times up to 10 h. The particle size was monitored and the chemical composition of the particles was studied with an Aerosol Mass Spectrometer and a Filter Inlet for Gases and AEROsols coupled with a Chemical Ionization Time-of-Flight Mass Spectrometer (FIGAERO-CIMS).

Particle evaporation was enhanced at higher RH with little change between 40% and 80%. Evaporation strongly depended on the initial particle composition, with lower volatility and a shift towards higher desorption temperatures in the FIGAERO thermograms (total ion count vs desorption temperature) for particles with higher O:C ratios.

Positive Matrix Factorization (PMF) was applied to the thermogram mass spectra data. The identified factors represent volatility classes which can be compared qualitatively to VBS distributions derived from other sources. Four to seven PMF factors were needed to reproduce the measured thermograms. Larger contributions of the low volatility classes were observed with increasing average O:C ratios. As expected from the thermograms, the residual particles after RTC evaporation contained a higher contribution of low volatility classes, but contrary to the expectation the average O:C ratio of the particles did not change with evaporation.

These results have important implications on our understanding of the fate of particles as they are transported and undergo further oxidation in the atmosphere. Higher oxidation levels and dry conditions make particles more resilient against evaporation and this need to be considered when predicting the climate effect of SOA with an equilibrium gas-particle partitioning model.

7AC.20

PRAPPE: Influence of Iron on the Photoaging of Particulate Matter in the Environment. FRANK LERESCHE, Joseph Salazar, David Pfotenhauer, Michael Hannigan, Brian Majestic, Fernando Rosario-Ortiz, *University of Colorado, Boulder*

Particulate Matter ($PM_{2.5}$) are produced by a variety of processes (e.g. from anthropogenic activities such as road emissions but are also emitted from natural sources) and are a particularly important research topic due to their detrimental impacts on human health. We present here investigations on the photoaging of these $PM_{2.5}$ in the aqueous phase and particularly on the influence of iron on the generation of hydroxyl radicals ($OH^•$) that are one of the major species driving to the photoaging of the $PM_{2.5}$. $OH^•$ being produced in PM extracts under irradiation through the Photo-Fenton reaction, nitrate photolysis and from the dissolved organic matter.

A sampling campaign called PRAPPE (Platte River Air Pollution and Photochemistry Experiment) investigating the properties of $PM_{2.5}$ coming from an urban, a rural and a mixed urban-rural site was done in the Denver area, Colorado. Characterization of the Iron speciation in the different sites as well as the measure of the total and soluble metals was the subject of another abstract. The focus of this abstract is on the photoaging mechanisms that drive the fate of $PM_{2.5}$ in aqueous phase and on the influence of Iron on the photoaging. The optical properties, such as the absorbance and fluorescence, and the capability of the $PM_{2.5}$ aqueous extracts to generate hydroxyl radical under simulated sunlight were investigated. Furthermore, the effects of solar irradiation were further explored by submitting the $PM_{2.5}$ extracts to simulated sunlight, artificially photoaging them. The observed light absorbance capacity was higher in the urban site than in the rural one and it was observed that the decrease in light absorbance properties during photoirradiation was correlated with the iron content of the extracts. The observations correspond to a scenario were the $PM_{2.5}$ are mostly produced in the urban site and are transported to the rural one, with a mean age of the $PM_{2.5}$ higher in the rural site.

This work should help to understand the parameters that influence the photoaging of $PM_{2.5}$ in the atmosphere, as well as the influence of trace elements on this process.

7AC.22

The Condensed-phase Ozonolysis of an Unsaturated Triglyceride: Reaction Kinetics and Products. ZILIN ZHOU, Shouming Zhou, Jonathan Abbatt, *University of Toronto, Canada*

Ozone plays an important role in both outdoor and indoor chemistry. It is well known that the gas-phase ozone oxidation of gas-phase alkenes, such as terpenes, leads to the formation of oxidized products, such as carbonyls and Criegee intermediates. However, despite the well-studied gas-phase mechanism, the fate of condensed-phase ozonolysis on surfaces and in aerosol particles is still not fully understood. In this study, a common component seen in most cooking oils, triolein (a triglyceride arising from glycerol and oleic acid) was oxidized by ozone on a surface. The rapid decay of triolein was observed, accompanied by the formation of secondary ozonides and a series of oxygenated compounds (acids and aldehydes). The uptake coefficient of ozone will be reported. To do this work, a sensitive technique using high-performance liquid chromatography/electrospray ionization mass spectrometry (HPLC-ESI-MS) was developed for the quantitative analysis of triolein and its oxidized products. In particular, the reactivity of the secondary ozonide products was also studied using this analytical method, under ambient conditions of light and relative humidity (RH). The results indicate that the condensed-phase oxidative chemistry of triglycerides is complex, driven primarily by the resulting Criegee intermediates. The environmental implications for this chemistry will be discussed. In particular, trigylcerides are an important component of cooking organic aerosol, and they will be deposited on indoor surfaces close to where cooking is performed.

7AC.23

Characterization of Aerosol Composition, Aerosol Acidity and Organic Acid Partitioning at an Agriculture-intensive Rural Southeastern U.S. Site. Theodora Nah, Hongyu Guo, Amy P. Sullivan, Yunle Chen, David Tanner, Athanasios Nenes, Armistead G Russell, Nga Lee Ng, Greg Huey, RODNEY J. WEBER, *Georgia Institute of Technology*

U.S. air quality regulations have led to decreased emissions in traditional air pollutants such as CO, NOx and SO2. In contrast, NH3 emissions have remained essentially unchanged, and may even increase in the future due to increased agricultural activities from a growing world population. These emission trends point to an increasingly important role that NH3 plays in atmospheric aerosol chemistry. We present real-time aerosol and trace gas measurements from a field study conducted in an agricultural-intensive region in Georgia during the fall of 2016. The goal was to understand how NH3 affects particle acidity and SOA formation via the gas-particle partitioning of semi-volatile inorganic and organic compounds. Particle pH and water were determined using the ISORROPIA-II thermodynamic model and validated by comparing predicted inorganic HNO3-NO3- and NH3-NH4+ gas-particle partitioning ratios with measured values. Our results showed that despite the high NH3 concentrations at the field site (study average 8.1 ± 5.2 ppb), PM1 are highly acidic with pH values ranging from 0.5 to 3.7 and a study-averaged pH of 2.1 ± 0.6 due to pH buffering by NH3 partitioning between the gas and particle phases. PM1 pH varied by approximately 1.4 units throughout the day. Gas-phase organic acids as large as C5 were detected at the site. Ambient concentrations of gas-phase organic acids ranged from a few parts per trillion by volume to several parts per billion by volume, with the largest concentrations observed for formic and acetic acids. Measured particulate organic acids comprised 6 % of the total organic aerosol mass concentration, with significant contributions from oxalic and succinic acids. The fractions of formic, acetic and oxalic acids present in the particle phase increased with PM1 pH. Measured formic, acetic and oxalic acid gas-particle partitioning ratios were also compared to their corresponding analytical predictions, which were calculated based on the organic acid's physicochemical properties, ambient temperature, particle water and pH. While the measured oxalic acid gas-particle partitioning ratios (fraction in the particle phase ranged from 39 to 88 % at pH between 1.2 and 3.3) generally agreed with analytical predictions, this was not the case for formic and acetic acids. Possible reasons for these disagreements will be discussed.

7AC.24

N2O5 Reactive Uptake and Chlorine Activation during Nocturnal Processing of Authentic Biomass Burning Aerosol.

LYDIA JAHL, Lexie Goldberger, Joel A. Thornton, Ryan Sullivan, *Carnegie Mellon University*

Nitryl chloride ($ClNO_2$) is a nighttime reservoir of NO_x that is formed from the uptake of dinitrogen pentoxide (N_2O_5) into particles containing chloride. $ClNO_2$ was thought to be formed only in the presence of chloride from sea spray aerosol, but its recent detection in areas far from the ocean has raised the possibility that other unrecognized particulate chloride sources make important contributions to chlorine activation chemistry. $ClNO_2$ is photolyzed each morning to produce the chlorine radical and recycle NO_x, thereby increasing the atmospheric oxidant budget. We recently demonstrated the production of $ClNO_2$ from heterogeneous reactions with $N_2O_5(g)$ under realistic conditions in a smog chamber reactor at Carnegie Mellon University. Iodide adduct chemical ionization mass spectrometry was used to measure gas phase $ClNO_2$ and N_2O_5, while a soot particle aerosol mass spectrometer measured changes in aerosol composition. Upon the addition of ozone to biomass burning smoke, N_2O_5 was consistently formed and $ClNO_2$ was subsequently detected in the gas phase. During experiments at high relative humidity, we observed decreases in particulate chloride and increases in particulate nitrate which we believe are due to acid displacement of HCl(g) by HNO_3 since no additional $ClNO_2$ was produced in the gas phase. The reactive uptake probability of N_2O_5 on authentic biomass burning aerosol and the yield of $ClNO_2$ were determined for the first time using flow tube experiments on smoke from biomass fuels including wiregrass, black needlerush, saw palmetto, and longleaf pine needles. Despite significant differences in aerosol composition, similar low reactive uptake coefficients were determined, in the range of 0.002-0.006. We investigated the controlling role that the aerosol particles' morphology and chloride mixing state play in the reactive uptake of N_2O_5 through single-particle analysis. N_2O_5 reactive uptake and the yield of $ClNO_2$ vs. HNO_3 were parameterized as a function of aerosol composition and mixing state, for incorporation into chemical transport models.

7AC.25

High Abundance of Oxalic Acid in a Rural Atmosphere of Eastern Central India: Influence of Biomass Burning and Photochemical Processing. DHANANJAY KUMAR DESHMUKH, Manas Kanti Deb, Kimitaka Kawamura, Dharmendra Kumar Singh, *Chubu University, Japan*

Organic aerosols (OAs) are abundant in the troposphere and crucial for air quality and climate. The oxidation products of OAs are highly water-soluble and typically contain several functional groups. Fine aerosol samples (PM2.5) were collected at a rural site of eastern central India (Ambikapur: 23.12°N and 83.20°E) during March to June 2017. The samples were analyzed for water-soluble dicarboxylic acids (C2-C12), glyoxylic acid (ωC2), glyoxal (Gly) and methylglyoxal (MeGly) as well as organic carbon (OC), elemental carbon (EC) and water-soluble OC (WSOC). Oxalic acid (C2) was detected as the most abundant species followed by succinic (C4) or malonic (C3) acids. The temporal variability in concentrations of C2 diacid and related compounds was pronounced during the end of March to the middle of April when biomass burning episodes were dominant in eastern central India. The strong correlation of C2 with levoglucosan ($r = 0.91$) suggests that biomass burning was a major source of oxalic acid in eastern central India. Strong correlations of the C2 with saturated diacids (C3-C9: $r = 0.81$-0.96), ωC2 ($r = 0.95$), Gly ($r = 0.92$) and MeGly ($r = 0.80$) suggest their similar sources and formation processes and that oxalic acid in fine aerosols may be secondarily produced from these precursor compounds. The ratios of WSOC to OC (0.52-0.88) and C3 to C4 diacid (0.69-1.30) suggest that water-soluble organic aerosols (WSOAs) were photochemically processed during the campaign. Our results demonstrate that severe biomass burning and photochemical processing enhanced abundances of WSOAs in a rural atmosphere in eastern central India.

7AC.26

In-situ Surface Tension Measurements of Hanging Droplet Aerosol Mimics under Photooxidative Conditions. Thomas Beier, JOSEPH WOO, *Lafayette College*

Oligomeric products of carbonyl-containing volatile organic compounds (CVOCs) have been shown to exhibit surface-active properties in aqueous aerosols, affecting their contributions to indirect radiative forcing effects on the atmosphere. These aerosol-phase oligomeric products are also known to exhibit compositional changes due to photobleaching in UV-irradiated environments. The relative rates of formation and effects of these oxidized compounds may be enhanced in aerosol conditions compared to in bulk phase due to their relatively high surface area, where these surface-active substances are thought to partition. In this study, surface tension and UV/Vis spectrographical data is collected for small (<20uL) hanging-drop aqueous aerosol mimics, which are exposed to controlled gas-phase CVOCs and UV radiation. These droplets act as an intermediate size scale between bulk mimic and aerosol-chamber studies, allowing for direct individual droplet measurement while maintaining a relatively high surface-volume ratio for heterogeneous photochemistry to occur. Observed surface tension and absorbance measurements are compared to Syszkowski-Langmuir and bulk-phase absorbance estimations (respectively) using GAMMA, a 0-dimensional computational box model.

7AC.27

Assessment of the Influence of Cut-Off Shift Due to Particle Hygroscopic Growth on the Analysis of Its Chemical Composition.

YING CHEN, Oliver Wild, Yu Wang, Liang Ran, Monique Teich, Johannes Größ, Lina Wang, Gerald Spindler, Hartmut Herrmann, Dominik van Pinxteren, Gordon McFiggans, Alfred Wiedensohler, *Lancaster Uni. and TROPOS*

Particulate matter is of major concern in the world nowadays, due to its effects on public health and climate. The chemical composition of particles is a crucial factor in these effects. Filter sampling is one of the major ways to measure aerosol compositions. However, the cut-off size for particle sampling shifts in different ambient conditions due to hygroscopic growth. This leads to difficulties in consistent comparisons between measurements under different conditions (spatial and temporal). This problem cannot be easily solved by drying airflow, since there is no efficient way to dry it for a high-volume aerosol sampler; moreover, the drying or heating processes change the gas-particle equilibrium and lead to a loss of semi-volatile compounds (e.g. nitrate and secondary organic aerosol). Here, we propose a method to assess this influence based on κ-Köhler theory (Petters and Kreidenweis, 2007). A global perspective on this influence is reported. This study is important for a consistent analysis of the long-term characteristics and spatial distributions of particle chemical compositions, and brings more confidence to model validation.

To explore the cut-off shift in filter-based particle sampling due to hygroscopic growth, we calculate the aerodynamic diameter of ambient particles based on the hygroscopic growth factor (GF) of size. The GFs are derived from κ-Köhler theory, with consideration of particle composition and size as well as meteorological conditions. The κ value, representing the dependence of particle hygroscopicity on chemical composition, can be estimated with composition measurements following the Zdanovskii-Stokes-Robinson mixing rule and Liu et al. (2014). Here, we adopt the previous reported global distributions of κ value (Pringle et al., 2010), relative humidity (RH, Dai, 2006) and temperature (Willett et al., 2014) to estimate the GF of particles in different sizes. The particle volume size distributions (PVSD) of eight different aerosol types (Whitby, 1978) are used to assess the influence of cut-off shift on chemical analysis.

Generally, European background sites seem to be more greatly influenced by the cut-off shift than those in other continents, with 10-20% in median and may reach 50-60% in some cases when hygroscopic particles present in humid air mass. However, the influence is generally much smaller (less than 7%) at all urban sites, and is negligible for hydrophobic dust particles. Sea salt aerosol (SSA) experiences the largest influence (about 50% in median), resulting from their large size, high hygroscopicity and high RH in marine air masses. A difference of more than 30% in the influence on SSA sampling can be observed between relatively dry and humid conditions. This work highlights importance of considering cut-off shift in chemical analyses when compare between different spatial/temporal conditions.

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7AC.28

Size-Resolved Physicochemical Properties of Organic Salt Nanoparticles. Sabrina Chee, Michael Lawler, Kelley Barsanti, Bryan Wong, JAMES SMITH, *University of California, Irvine*

The volatility and hygroscopicity of atomized alkylaminium carboxylate particles have been previously studied in laboratory experiments. However, these properties have not been measured for nanoparticles formed from the acid-base reaction between gas-phase alkylaminium bases and organic acids. To study this, gas-phase acetic acid (CH_3COOH) and dimethylamine (DMA) were introduced into a flow tube reactor to nucleate and grow nanoparticles (defined here as < 50 nm) under dry and elevated relative humidity conditions. A Thermal Desorption Chemical Ionization Mass Spectrometer (TDCIMS) was used to measure the size-resolved chemical composition of the nanoparticles formed, and volatility and hygroscopicity measurements were taken by using Volatility and Hygroscopicity Tandem Differential Mobility Analyzers (H- and V-TDMAs, respectively).

Acid:base ratio measurements from TDCIMS are presented. Size-resolved volatility measurements suggest that dimethylaminium acetate nanoparticles are less volatile than ammonium sulfate nanoparticles of comparable sizes and temperatures. These results are combined with thermodynamic modeling to explore the limits of bulk thermodynamic properties of acids and bases, such as pKa, in determining the size-dependent acid:base ratio of the dimethylaminium acetate nanoparticles formed. The implications of these modeling observations on alkylaminium carboxylate nanoparticle volatility are also discussed.

7AC.29

Physical and Chemical Submicron Aerosols Properties and Their Link to Size-resolved Aerosol Hygroscopicity in Summer/Spring of Seoul, Korea. NAJIN KIM, Minsu Park, Seong Soo Yum, Hye Jung Shin, Jong Sung Park, Joon Young Ahn, *Yonsei University*

Hygroscopic behavior of aerosols are important parameter of climate change and air quality as aerosol hygroscopicity is not only connected to cloud condensation nuclei (CCN) activity but also to the visibility in highly polluted areas. It is widely known that aerosol hygroscopicity is closely related to physical and chemical properties of aerosols. In this study, characteristics of submicron aerosols and their links to aerosol hygroscopicity are examined based on the results of KORUS-AQ (May-June, 2016) and MAPS-Seoul (May-June, 2015) campaigns, which aims at understanding various aspects of air quality problem in Seoul, highly urbanized area in Korea. Size-resolved aerosol hygroscopicity were measured by hygroscopic tandem differential mobility analyzer (HTDMA) and analyzed with data from various instruments for measuring physical and chemical aerosol properties: CPC, SMPS, CCNC, HR-ToF-AMS and MAPP.

Distinct diurnal patterns of size-resolved aerosol hygroscopictiy and mixing state were observed during the measurement periods. In the morning, aerosols are externally mixed with freshly emitted particles by vehicles and existing aged aerosols. Mixing state change occurred in the afternoon when photochemical process is active. Sharply increased hygroscopicity of small particles and O/C ratio were observed in that time. During KORUS-AQ campaign, chemical composition of aerosols varied by sources (inorganic-dominant/ organic-dominant period) and impacted on aerosols hygroscopicity and even CCN spectrum even though aerosol number concentration changed very little. Good agreement with GF-derived κ from HTDMA and AMS-based κ when considering oxidation state and BC mass concentration also implies that hygroscopic properties of aerosols are associated with chemical properties of aerosols as well as physical properties of aerosols. Analysis of aerosol chemical composition with size-resolved aerosol hygroscopicity during NPF events and difference between GF-derived κ and CCN-derived κ will be discussed in the conference.

7AC.30

Aerosol Acidity Measurement Using Colorimetry Coupled with a UV-Visible Micro-spectrometer and Its Application to Measurements of Organosulfates in Ambient Air.

SHIQI SUN, Myoseon Jang, *University of Florida*

Although SO_2 concentration has been reduced in USA for last two decades, the acidic aerosol produced from the oxidation of SO_2 is still an existing problem in many countries (i.e., Asia and South America) who rely on coal for heating and industries. Sulfate significantly contributes to total fine particulate matter, and yet the prediction of aerosol acidity remains inadequate. Atmospheric aerosol acidity influences the health effects of particulates due to metal solubility, and is also a kinetic model parameter that processes acid-catalytic reactions of atmospheric organics and organosulfate formation to increase secondary organic aerosols. Our laboratory's recent research efforts have improved the state-of-the science-art via the development of colorimetry integrated with a Reflectance UV-Visible spectrometer (C-RUV). In this study, a portable C-RUV device in the field is developed using a micro-spectrometer that is self-contained and deployable. The C-RUV technique operates by passing an air sample through a filter infused with an indicator (i.e. metanil yellow), which changes color in response to acidity changes. The optical probe transfers both the source beam from the micro-spectrometer to the filter surface through the optical fiber, and the reflected beam from the filter to the detector in the micro-spectrometer. The proton ($[H^+]$, mol/L of aerosol) measurement by the C-RUV method has been calibrated for inorganic aerosols comprised of ammonium and sulfate under varied humidity conditions using a flow tube. The resulting C-RUV device and the calibration equation are applied to quantify $[H^+]$ in the ambient air. The acidity aerosol can be modulated by both neutralization of sulfuric acid with ammonia and the formation of organosulfate in aerosol. The concentration of organosulfate in aerosol is also estimated by using the difference in proton concentrations obtained from C-RUV and a particle into liquid sampler ion chromatography (PILS-IC) in ambient air. The aerosol acidity measurement using C-RUV device is able to improve the modeling of aerosol formation and the prediction of aerosol hygroscopicity.

7AC.31

Simultaneous Water Uptake and Size-resolved Bounce Measurement of Secondary Organic Aerosols. DEVOUN STEWART, David De Haan, Richard Gardner, *University of San Diego*

The phase change of secondary organic aerosols in the atmosphere is of significant scientific interest because of its effects on climate. The effect of aerosols on climate is closely linked to aerosol interaction with water. Solid aerosols can uptake water under humid conditions, which causes them to liquefy. Under these conditions, the optical properties of aerosols, which depends on its size and phase, will change. The light scattering properties of aerosols increase significantly when particle absorbs water. Since the climate effects of aerosols are closely tied to interactions with water, we developed an instrument capable of simultaneous aerosol water uptake and size-resolved bounce measurements. This instrument uses two SMPS system connected to a MOUDI impactor to simultaneously measure both particle growth and bounce factors at various controlled relative humidity. The size-resolved bounce measurements allow us to determine how much water uptake is required for the aerosol to liquefy. In this presentation, we will present results of the size-resolved phase change and growth factors of different secondary organic aerosols. Our instrument was validated by measuring the growth and bounce factor of ammonium sulfate aerosols.

7AC.32

Temporal Variability of Fine Particle Liquid Water Content over a National Park in Central India. SAMRESH KUMAR, Ramya Sunder Raman, *Indian Institute of Science Education and Research, Bhopal*

Aerosol liquid phase water (ALW) is an important component of ambient aerosols. Water condensed on aerosols promotes heterogeneous chemical reactions along with obscuring the visibility, altering the hydrological cycle and influencing regional climate. It also influences the atmosphere-biosphere interactions, transport, atmospheric processing and fate of trace species. ALW is dependent on relative humidity, temperature, aerosol composition and concentration.

This work focuses on understanding the impacts of relative humidity, temperature, aerosol composition and concentrations on ALW for different time scales. 12 hour integrated samples ($PM_{2.5}$) were collected over a National Park in Central India for two years (2012-2013, N=329; day and night) on multiple filter substrates using co-located Mini-VolTM samplers. Onsite metrological parameters were also recorded using Vaisala WXT-520 sensors. Water soluble inorganic ions in $PM_{2.5}$ were determined using Ion Chromatography while organic and elemental carbon were determined using the DRI Thermal Optical Transmittance/Reflectance analyzer. Inorganic ions along with metrological parameters (relative humidity, temperature) were used to calculate the ALW content. Results of ALW content calculated using the Extended Aerosol Inorganic Model (E-AIM) and κ-Köhler theory (organic particle water) will be presented.

7AC.33

Atmospheric Concentration of Polycyclic Aromatic Hydrocarbons (PAHs) and Nitro- PAHs, Their Temperature Dependence and Gas to Particle Partitioning at a Traffic site in Agra, India.

PUNEET KUMAR VERMA, Dinesh Sah, Rangu Venkata Satish, Neeraj Rastogi, K. Maharaj Kumari, Anita Lakhani, *Dayalbagh Educational Institute, Agra 282005, India*

Sixteen priority and two Nitro-Polycyclic Aromatic Hydrocarbons was measured simultaneously both in the gas and particulate phase between October 2015 to July 2016 in the ambient air of Agra, India. Gas and particulate phase samples were collected using High volume sampler on Poly urethane foam plugs and Quartz micro fiber filter papers respectively. Samples were extracted in a mixture of DCM and n-hexane and further analysed using Gas Chromatograph coupled to a Mass Spectrometer. During the sampling period the average total PAH concentration in particulate phase and gas phase were 3121 ± 308.9 and 1732.5 ± 175.1 ng m^{-3} respectively whereas the concentration of Nitro PAHs was 65.3 ± 16.3 and 24.6 ± 6.55 ng m^{-3} in the particulate phase and gas phase respectively. Gas particle partitioning of PAHs was investigated employing the Junge-Pankow adsorption, K_{OA} Absorption and Dual model. Statistically significant correlation ($p<0.001$) for log Kp vs log $P_{\underline{o}l}$ was obtained for individual PAHs. Temperature dependency of ambient concentration of PAHs was also investigated using Clausius–Clapeyron plots which suggests that concentration of high volatile PAHs is influenced by the temperature. Positive slope of log Kp and 1/T suggest that the density of PAHs (m^3 μg^{-1}) is directly proportional to ambient temperature. In health risk assessment DbA was found as the most carcinogenic and mutagenic as compared to other PAHs followed by BaP.

Key words: Polycyclic Aromatic Hydrocarbons (PAHs), Nitro-PAHs, Junge-Pankow adsorption model, K_{OA} absorption model, Dual model.

7AC.34

New Methods for the Study of the Effects of NOx on SOA Formation. WEIHAN PENG, David R. Cocker III, *University of California, Riverside*

NOx effects are important on SOA formation in atmosphere since both low vapor pressure species formed in peroxide rich (low-NO) conditions and organic nitrate formation in higher NOx environments affect aerosol formation. Current regional air quality models, when considering NOx effects, are guided by results from classic environmental chamber experiments, most of which explore the influences of initial NOx concentration on final SOA formation. During most of these experiments, significant SOA formation does not start until the NO in the system is depleted through oxidation to NO2 and such experiments might have multiple NOx regimes regardless of the absolute amount of NOx injected, so they may miss important SOA formation pathways leading to errors to these models. Therefore, it is important to design new methodologies to study NOx effects at different regimes in environment chamber to provide a more accurate guidance to air quality models. In this study, instead of completing the precursor VOCs and NOx injections before the start of SOA formation like it is in traditional chamber experiments, the timing and method of VOC precursors and NOx are altered in the current work to enhance and simulate the conditions for peroxide and organic nitrate formation. Varied amounts of NOx were injected after the SOA formation commences to explore its effects in peroxide rich environments. Different injection methods including continuous and step-wise injection were conducted to study the instantaneous effects. Additional experiments were performed with precursors VOCs injected after depletion of NO to study NOx effects in low NO conditions.

This study presents experimental observations from the photo-oxidation systems of major anthropogenic VOCs (e.g., aromatics), biogenic monoterpene and poly-aromatic hydrocarbons. Experiments were conducted in the dual 90m3 environment chamber at UCR/CECERT and modelling of gas-phase chemical reactions were guided by the SAPRC model gas-phase chemical mechanism along with measurements of gas species including ozone, NOx, VOCs, aerosol number and volume time traces as well as aerosol density, volatility and bulk chemical composition. For the same total NOx injected, the timing of the NOx injections significantly influenced the SOA formation in the system by altering the gas-phase chemical reactivity of the system that the VOC precursor reacted in. Changes in SOA formation along with chemical and physical characteristics of the resulting aerosol will be discussed.

7AC.35

Volatility and Chemical Characterization of Secondary Organic Aerosols Formed from Aqueous-Phase Oxidation.

SARAH SUDA PETTERS, Barbara Turpin, *University of North Carolina at Chapel Hill*

Oxidized organic matter makes up a large fraction of the global aerosol burden and exerts an important influence on regional climate, human health and wellbeing, and the visibility of distant landmarks. Secondary organic aerosol (SOA) is formed when organic gases are oxidized and their reaction products condense. Condensed organic matter formed from the aqueous oxidation of water-soluble organic gases in cloud droplets and wet aerosols is increasingly recognized to be an important SOA contributor. However, quantifying the contribution of aqueous-phase mechanisms to SOA remains challenging. A major variable in determining aerosol yield is the volatility of the reaction products of aqueous-phase oxidation. A more detailed understanding of reaction products and their volatility is needed. Here we present the experimentally-determined volatility of SOA produced by aqueous oxidation of several precursors including pyruvic acid and methyl vinyl ketone. Oxidized organic matter was produced in a batch reactor containing an aqueous mixture of dissolved precursor and hydrogen peroxide. OH radicals were produced by photolysis of the hydrogen peroxide through ultraviolet irradiation. Samples were collected at intervals and chemical characterization was performed using ion chromatography (IC) and quadrupole time-of-flight mass spectrometry (QTOF-MS). Volatility was determined by pumping the sample through a vibrating orifice aerosol generator (VOAG), which produces a stream of monodisperse droplets of known size. Water and volatile compounds were evaporated at 20 degrees C and the particle residual volume was determined by an optical size spectrometer. The volume fraction remaining was determined by comparison of droplet residuals to the total organic carbon (TOC) in each sample, and volatility was estimated by comparison to calibration experiments using compounds of known volatility. Results show the dependence of volatility of aqueous oxidation products on concentration and on perturbations in solution pH made by the added presence of ammonium. Of particular interest are the volatilities of pyruvic acid aerosols in the context of the mechanisms of both pyruvic acid formation in the atmosphere and of aqueous aerosol formation from pyruvic acid. Recommendations for further investigation are discussed.

7AC.36

Comparing Organic Speciation of Biomass Burning Aerosol Produced in Laboratory Burns and Prescribed Fires in the Field. AUDREY DANG, Skyler Simon, Claire Fortenberry, Michael Walker, Christopher Oxford, Benjamin Sumlin, Jiayu Li, Jonathan Myers, Brent Williams, *Washington University in St. Louis*

Both laboratory and field measurements of chemical source profiles contribute to our understanding of organic aerosol, which negatively affects human health and impacts global radiative forcing. While laboratory experiments allow more careful control of sources, field measurements capture realistic emission conditions. For example, the chemical composition of biomass burning organic aerosol depends on combustion phase (e.g., flaming or smoldering) as well as the fuel type (e.g., oak or lodgepole pine, leaf or heartwood), making supporting laboratory experiments necessary to differentiate contributing source types and combustion conditions in complex field observations (Fortenberry et al. 2017).

We compare organic speciation of biomass burning organic aerosol sampled during prescribed fires of forest plots at Tyson Research Center (30 km southwest of St. Louis, MO, USA) and produced during laboratory burns of biomass collected from the same plots. Both laboratory and field samples are collected on quartz filters for analysis with a Filter Thermal Desorption Aerosol Gas Chromatograph (Filter TAG). Field samples were collected below the canopy as well as above the canopy with an unmanned aerial vehicle. Individual molecular markers and positive matrix factorization (PMF) solutions of binned chromatograms are compared (Zhang et al. 2014).

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7AC.37

Characterizing the Thermal Desorption Behavior of Hemiacetal and Acetal Oligomers. MEGAN CLAFLIN, Paul Ziemann, *University of Colorado*

The presence of oligomers in atmospheric aerosols has been observed both from field measurements and for particles formed in laboratory experiments. The formation of these compounds has been attributed to particle-phase accretion reactions that occur on timescales that range from seconds to a few hours. Common types of oligomers that are formed in aerosols include hemiacetals, acetals, and peroxyhemiacetals. While the existence of these compounds in aerosols has been verified, their detection using preferred methods by the atmospheric community, such as online mass spectrometers that utilize thermal desorption, can be difficult due to decomposition or fragmentation. Thermal desorption methods, like the FIGAERO-CIMS, offer the opportunity to detect compounds separated by their volatility. Yet how oligomers, especially those that form via reversible reactions, respond to thermal desorption is unclear. There has been evidence that under some conditions, the thermal ramping can cause the oligomers to revert to their monomer building blocks, and thus when detected they would not reflect the true aerosol composition.

To study the effects of thermal desorption on hemiacetals and acetals, both synthesized standards and the SOA formed from the reaction of β-pinene with NO_3 radicals were investigated. Previously, we have shown that >90% of the β-pinene SOA is made up of hemiacetal and acetal oligomers. Therefore, this system provides an opportunity to look at the thermal desorption properties of real SOA that has been carefully characterized and is made almost entirely of oligomers.

The thermal desorption behavior was studied using two types of mass spectrometers. The first was a Temperature Programmed Thermal Desorption Particle Beam Mass Spectrometer (TPTD-PBMS) which uses electron ionization and a thermal desorption ramp rate of 2 ^{0}C min^{-1}. This instrument was used to study how these classes of compounds are ionized in real time, by instantaneous vaporization, versus how they behave when slowly desorbed by heating. The second was a Chemical Ionization Ion Trap Mass Spectrometer (CI-ITMS) equipped with a Direct Insertion Probe (DIP) that uses a thermal desorption ramp of 10 ^{0}C min^{-1}, a ramp rate that is comparable to that used with the FIGAERO-CIMS.

The results of our experiments show that when hemiacetals are analyzed in real time they are ionized as the intact oligomer. However, when they are slowly heated using a thermal desorption method the hemiacetals decompose and are instead ionized as their monomers. This effect was not seen for acetals, which were ionized as the intact oligomer for both real time and thermal desorption analyses.

Our intention of characterizing how these types of oligomers respond to thermal desorption detection methods is to give insight on the interpretation of data for aerosol systems that are likely to contain these classes of compounds. Without accounting for decomposition of oligomers, the consequence is likely misassigning the volatility of an aerosol and thus misrepresenting the physical properties of the particle.

7AC.38

Gas-particle Partitioning and Temperature: Competition Between Vapor Pressure Dependence and Phase-state. CHEN LE, Weihan Peng, Mary Kacarab, David R. Cocker III, *University of California, Riverside*

Secondary Organic Aerosol(SOA) formation potentials from Volatile Organic Compounds(VOC) precursors are often described assuming that partitioning species are at thermodynamic equilibrium as is the case in the classic two-product SOA partitioning model and in the volatility basis-set model. Temperature dependence on SOA formation following these models can then be estimated using the Clausius-Clapeyron vapor-pressure temperature dependence relationship and an assumed enthalpy for the condensable species. Describing gas-particle partitioning using this model assumes: 1) temperature change in the system does not alter the composition in the system; 2) that equilibrium within the system is rapidly achieved. Therefore, it should be expected that the temperature of the system will determine gas-particle partitioning equilibrium regardless of the temperature that oxidation occurred at.

Observations in the CE-CERT environmental chamber over the past decade demonstrate: 1) far more aerosol is formed in systems operated at 5ºC and then warmed to 25ºC than in systems operated at 40ºC and cooled to 25ºC, even after accounting for chamber wall effects; 2) gas-particle partitioning cycling between temperatures for a single experiment regardless of initial temperature, however, is reversible and can be described applying an either empirical or semi-empirical enthalpy of vaporization.

This study discusses these apparent observational anomalies. The effect of aerosol-phase state and viscosity is evaluated using the dual-differential mobility analyzer technique described by Rothfuss and Petters (2016) in the dual-Teflon indoor chamber at CE-CERT. The technique induces coagulation between two oppositely charged particles and relates viscosity to the relaxation time for the dimer to return to a spherical shape. The effect of phase-state along with chemical kinetics at the different experimental temperatures are used to explain the apparent non-equilibrium temperature effects observed. Strong relaxation time temperature dependencies were observed during environmental chamber temperature shifts that suggested that mass-transfer related kinetic effects were responsible for the irreversibility observed between gas-particle partitioning of SOA formed at 5ºC and 40ºC. This work focuses on observations of temperature effects from the α-pinene dark ozonolysis and m-xylene – NOx photooxidation system including gas-particle partitioning and changes to chemical composition.

7AC.39

Exploration of Potentially Increasing SO2 Oxidation in the Eastern United States. BRET SCHICHTEL, Anthony Prenni, Jenny Hand, Scott Copeland, Kristi Gebhart, John Vimont, William Malm, Jeffrey Collett, *National Park Service*

In the early 1990s, ammoniated sulfate accounted for about two-thirds of the fine particulate mass in the rural eastern U.S. as measured by the Interagency Monitoring of Protected Visual Environments (IMPROVE) program. Particulate sulfate also had a distinct seasonal cycle, with summer concentrations a factor of 2 larger than in winter. In the ensuing 25 years, sulfur dioxide (SO2) emissions have decreased by about a factor of 10, resulting in well-documented decreases in SO2 measured by the Clean Air Status and Trends Network (CASTNET) program and particulate sulfate measured by the IMPROVE and CASTNET programs. The reductions in particulate sulfate were commensurate with the SO2 emission reductions until about 2008, when the trends diverged, after which time smaller decreases in particulate sulfate occurred for every unit decrease in SO2 emissions. The ratios of ambient sulfate to SO2 also increased in CASTNET measurements. In addition, particulate sulfate seasonality was substantially reduced throughout the eastern U.S. One explanation for this recent nonlinear response of particulate sulfate to changes in SO2 emissions is that the SO2 to sulfate oxidation may have become more efficient, resulting in a greater fraction of SO2 being converted to sulfate. Alternatively, these observations may be driven by increased background sulfate concentrations from international sources or primary emissions of particulate sulfate. In this presentation we will explore these possible causes and present the available evidence suggesting that the fraction of SO2 oxidized to sulfate in the eastern U.S. has increased over the past 10 years.

7AC.41

Trends in Organic Aerosol Mass and Functional Group Composition in the SouthEastern Aerosol Research and Characterization (SEARCH) Network from 2008 to 2016. ANN DILLNER, Alexandra Boris, Andrew Weakley, Bruno Debus, Eric Edgerton, Stephanie L. Shaw, Satoshi Takahama, *University of California, Davis*

Organic aerosol (OA) concentrations are on the decline in the Southeastern US. This presentation covers trends in OA and its composition as described by organic functional groups at five sites in the Southeastern Aerosol Research and Characterization (SEARCH) Network over a recent 9-year period. Functional groups are estimated in particulate matter (PM) filter samples using a Fourier transform infrared spectroscopy (FT-IR) technique. The vast filter archive of SEARCH samples, stored cold since 2008, enables the application of FT-IR to nearly a decade of aerosol samples at two urban-rural paired sites and a coastal site. OA contains thousands of molecules, but typically only ~5-30% of OA mass is identified in atmospheric PM composition studies. However, in this work FT-IR functional group measurements enable the quantification of nearly all OA sample mass. In addition to describing trends in OA composition, we will estimate the ratio of organic matter to organic carbon concentration (OM/OC) in each analyzed sample to provide a metric for aerosol oxidation and to provide a tool for converting routinely measured OC concentrations to OM.

The contribution of carbonyl, carboxylic acid OH, aliphatic CH, and alcohol OH to OA mass are measured at two urban/rural pairs (i.e. Atlanta and Yorkville, GA; Birmingham and Centreville, AL) and a coastal site in Florida from 2008 to 2016. To measure functional groups, laboratory standards are made by aerosolizing compounds containing each functional group and collecting them on PTFE filters using a SEARCH sampler. The laboratory standards are analyzed by FT-IR, and the resulting infrared spectra are used to develop partial least squares calibration models. The calibration models used in this study expand upon previous work to include a broader, more atmospherically relevant selection of chemicals. This includes chemicals representing oxidation products such as multifunctional carboxylic acids and a tetrol, carboxylate salts demonstrating interaction between inorganic and organic species, levoglucosan to represent biomass burning emissions, and an amino acid to represent the contribution of reduced organic nitrogen species. This work better quantifies carbonyls in particular, as compared to prior work. This work also demonstrates the spatial and seasonal variability and trends in functional groups and OM/OC within the diverse and abundant OA collected in the SEARCH network.

7AE.1

Investigation of Ground Level Aerosol (PM2.5) with Different Mode of Transports in Dhaka, Bangladesh. AHMAD MAJUMDER, M.D. Hossain, Abdullah Nayeem, *Stamford University Bangladesh*

Air pollution is considered as a threat to the environment of the modern cities. The study was carried out through the field experiments, collection and analysis of data from both primary and secondary sources to determine the concentration of particulate matter and causes of pollution.The study reviewed the suspended solid particulates specifically $PM^{2.5}$ and compared between different categories roads which are Non-motorized, Mixed and Motorized and also with Environment Quality Standards (EQS) for Bangladesh published by the Department of Environment (DoE).This study outlinesalso make a co-relation between concentration of the particulate matters and increasing of motorization.$PM^{2.5}$ was measured and conducted traffic volume survey in 12 sites across the city in Dhaka (August 2017). Levels in mixed and motorized areas were on average 182 and 272% higher, respectively, than non-motorized. Surprisingly, short term measurements (~8hrs) in predominantly mixed and motorized areas already exceeded the maximum recommended limit for 24hrs (65 $\mu g/m^3$). This suggests a much higher pollution potential over a typical 24hrs period in motorized traffic areas. The study hypothesized that uncontrolled motorization is major cause of air pollution especially $PM^{2.5}$ in the Dhaka city and the impact of these particulate matters on public health and environment are beyond the tolerable limits.The study has come up with some recommendations regarding improvement of air quality in respect of particulate matter and emphasized for further comprehensive study on other parameters of air pollution around Dhaka city.The study drew conclusion that the overall air quality regarding the particulate matter already exceeded highest standard limits of Bangladesh. The study recommended several measures to mitigate and prevent the harmful impacts and to improve the air quality of Dhaka city.

Key Words: Pollutant, Air pollution, Motorized, Non-motorized, Human health.

7AE.2

Health and Economic Effects of Wildfire in US. KAIYU CHEN, Hao Guo, Hongliang Zhang, *Louisiana State University*

Nowadays wildfire is the largest source of air pollutants that greatly changes landscape with impacts on human health, large scale climate changes, social economy and ecosystem in the U.S. The Community Multi-scale Air Quality (CMAQ) model is applied to simulate potential impacts on air pollutants due to wildfire in 2011. The National Emissions Inventory (NEI) 2011 is used to generate anthropogenic emissions with the Sparse Matrix Operator Kernel Emissions (SMOKE) emission processing model. The wildfire emissions are generated based on the fire inventory from National Center for Atmospheric Research (NCAR). Contributions of wildfires to air pollutants concentrations are quantified and the estimate health and economic outcomes are estimated using the US EPA developed Environmental Benefits Mapping and Analysis Program (BenMAP). Premature mortality, non-fatal heart attacks, aggravated asthma and economic risk are estimated to represent impact of wildfire and help to improve air quality controlling strategy.

7AE.3

Quantifying the Impact of Wildfires on Air Quality and Human Health: the Case of Equatorial Asia. PAOLA CRIPPA, Stefano Castruccio, Mohd Talib Latif, M.S.M. Nadzir, D. Dominick, Mikinori Kuwata, Abhinav Thota, M.I. Mead, Christine Wiedinmyer, *University of Notre Dame*

Forest and peat fires have become a frequent occurrence in Equatorial Asia as a result of a warmer and drier climate, uncontrolled agricultural practices and intentional ignition. Air pollutants from wildfires, including carbon monoxide (CO) and particulate matter (PM), can be transported in the atmosphere for thousands of kilometers from the originating fires and thus significantly impact air quality and human health over wide areas. In this work we focus on the extreme fires occurred in Fall 2015 in Equatorial Asia and assess air quality conditions and associated population exposure. Quantifying the impact of wildfires on human health is currently limited by the lack of integrated studies including both direct Earth observations, modeling tools and health records. In our study we apply a state-of-the-art regional model (WRF-Chem) at high spatio-temporal resolution to characterize air pollution episodes from the 2015 wildfires in Equatorial Asia. Simulated PM and CO concentrations are evaluated against satellite observations and data from a dense ground-based network and indicate high skills of WRF-Chem in capturing both the spatio-temporal variability and magnitude of these events. We estimate that, during September and October 2015, 69 million people were persistently exposed to unhealthy air quality conditions. Further, the short term exposure to the enhanced PM2.5 concentrations from wildfires may have caused 11,880 (6,153–17,270) excess mortalities. Our results indicate that by using a high resolution regional model we can provide unique information to policy makers to coordinate the effort between emitting and exposed countries in improving air quality and reducing population exposure.

7AE.4

Spatially-Resolved Comparison of Traffic and Cooking-Related PM1 Emission in Urban Area and Their Threat to Public Health. Peishi Gu, Zhongju Li, Qing Ye, Ellis Shipley Robinson, Joshua Apte, Allen Robinson, ALBERT PRESTO, *Carnegie Mellon University*

Spatial gradients of PM1 concentration (particulate matter under 1 mm in diameter) have been discovered near local sources, such as highways and restaurants, etc. The population that lives or works in these impacted regions is often exposed to higher than background PM concentration, and this may increase their short-term and long-term health risks. From a perspective of regulation, it is essential to understand what sources are responsible for the elevated concentration, and how are population impacted by the sources spatially. In this study, we have utilized a mobile sampling platform coupled with HR-ToF-AMS and Aethalometer to investigate the spatial distribution of PM1 in Pittsburgh, which is a major city in the northeastern United States. We performed extensive mobile measurement in areas of various types of land-use. Cooking and traffic-related organic aerosol (OA) were resolved as the major primary sources by positive matrix factorization (PMF). We included the spatially resolved statistics of traffic volume, restaurant counts and population, and performed GIS analysis based on a 200-meter grid overlay on the sampling domain. We have found that more than 80% of the population is located within the 200-meter range of identified local sources, and the existence of such sources are strongly associated with the elevated PM1 concentration. For OAs, cooking is more important compared to traffic as a primary source, based on both the concentration and the impacted population. However, since diesel engines dominate the emission of black carbon in urban areas, traffic source still poses a greater threat to public health than cooking.

7AE.5

Efficiency of Anti-Pollution Masks in Three Microenvironments. BORIS GALVIS, Camila Figueredo, Fabian Moreno, Jorge Pachon, *Universidad de La Salle*

We tested different commercially available masks to determine the reduction in exposure and dose of fine particulate and black carbon that each might provide. We evaluated them inside the Bogota's BRT buses, on a pedestrian route in the city's downtown area and on a bike path using two sets of DustTrack DRX (TSI, Shoreview, MN) and AE51 microaethalometer (AethLabs, San Francisco, CA). One set sampled air directly from the microenvironments whereas the other did it through the masks. We used a mannequin head as an adapter for the masks to the inlets of the instruments and to take in to account how the masks fit. Both sets operated simultaneously and concentrations measured were used to estimate a possible reduction in exposure and potential inhaled dose of aerosols. Results might be used to show citizens how to reduce their exposure during commutes in a megacity and to point towards the most effective way to prevent effects during an air pollution episode.

7AE.6

Air Quality with Particulate Matter Assessment in Road Tunnels in China and Pakistan. ZONA ZAIDI, Zulfiqar Ali, Romaisa Qureshi, Irfan Zainab, Syed Turab Raza, Zaheer Ahmad Nasir, Ian Colbeck, Liu Weilong, *University of the Punjab, Lahore, 54590, Pakistan*

Breathing in road tunnels may endanger your health. Poor air quality on roads and in tunnels threatens the health and well-being of people travelling in vehicles. Air pollutant in road tunnels could be in the form of a solid particle, liquid droplets or as gases. The objective of this research was to assess air pollution in 44 road tunnels of China i.e., Chengdu to Lang Musi Zhen (32°39'35N, 103°36'09E at 2876m elevation) and 5 tunnels of Pakistan i.e., Shishkat to Attabad (36◦39.747N, 074◦50.586E at 2839m elevation). Metrological parameters, CO_2 concentration along with different particulate matter were assessed using standard protocol. Independent t-test showed PM_1, $PM_{2.5}$, PM_{10} and PM_{total} concentrations for China and Pakistan were non-significantly different from each other with p-value 0.071, 0.069, 0.071 and 0.07 respectively while temperature, humidity and carbon dioxide were significantly different from each other having p-value 0.000, 0.000 and 0.011 respectively which are also justified by Pearson co-relation. Spearmen's correlation assessed relationship between different parameters and their associative behaviour and showed temperature was non-significantly correlated with particulate matter, humidity and CO_2. While $PM_{2.5}$, humidity and CO_2 were significantly correlated. CO_2 concentration as linear with vehicular emission was higher inside of tunnel in china but traffic blockage in Pakistan rise its high levels outside of it. The confinement of tunnel's air aided by its boundary along with massive traffic becomes the major factor in rise of temperature inside of tunnel along with humidity as water drops trap inside of it due to lesser air currents.

7AE.8

Emission of Particulate Matter, VOCs and PAHs from Different Asphalt Mixes. MENG XIU, Xianyu Wang, Jochen Mueller, Andrew Beecroft, Lidia Morawska, Phong Thai, *Queensland University of Technology*

Asphalt is widely used for road pavements across Australia, and is considered heavily resource intensive. On the other hand, in Australia, millions of tyres reach the end of their service life every year and need to be disposed of. New technology allows end-of-life tyres to be processed as crumb rubber and recycled in road construction as an additive to save materials and reduce waste, with the product known as crumb rubber modified (CRM) binder. However, application of asphalt mixes, including the CRM binder, can generate toxic fumes and emissions including those of total suspended particles (TSP), volatile organic compounds (VOCs) and polycyclic aromatic hydrocarbons (PAHs). These pollutants not only deteriorate air quality in the immediate vicinity, but also raise health risks to paving workers. Research outcomes regarding environmental and health issues associated with the application of CRM mix are still scarce.

This study, therefore, aims to compare the levels of air pollutants during pavement of different asphalt mixes including the CRM mix, as well as assess the risk for their emissions. Two field investigations were performed on several different construction site. Emission factors of TSP, VOCs and PAHs from different asphalt mixes were measured using portable flux chambers, connected simultaneously with a vacuum canister (for VOCs sampling) and two active air samplers (for TSP and PAHs sampling respectively). A total of 60 VOC analytes and 13 PAH compounds are analysed by a gas chromatography-mass spectrometer (GC-MS) and a gas chromatograph coupled to a high-resolution mass spectrometer (GC-HRMS), respectively. For personal exposure, a Dustmate device is provided to the workers (a paver driver and a screed operator) to monitor personal exposure to particulate matter (PM), including $PM_{2.5}$, PM_{10} and TSP, which may be inhaled via the respiratory pathway.

In the results of the field study 1, TSP levels were found to be 2.5 times higher for the CRM operation than PMB, and higher than the Queensland air quality objective. Apart from the appearance of some alkanes and naphthalene during the construction work, the levels of other VOCs are mostly below limit of report. Although there was an increase in the level of BaP and PAHs in the ambient air during and shortly after the construction, the highest concentrations measured (0 – 3 hrs after spray) in both treatments were much lower than the Queensland air quality objective. The results of the field study 2 showed that CRM hot mix was likely to produce higher concentration of air pollutants (VOCs and PAHs) than both CRM warm mix and polymer mix, even though no significant difference ($p>0.05$) was observed for levels of TSP, PM_{10} and $PM_{2.5}$ at work site. The data from this study is expected to contribute to the overall assessment of the comparative risk of using ground tyre rubber techniques in road paving industries in Queensland.

7AE.9

Assessment of Exposure to Bioaerosols and Heavy Metals in a Material Recovery Facility in Central Taiwan. HUI-MING LIU, *Hungkuang University*

Recently the world's energy and raw materials availability is progressively dwindling result in rapid development of the materials recycling industry. Bioaerosols and metal dusts are accompanied during materials recycling process and harm to human health. Hence, it is necessary to investigate the exposure to metals and bioaerosol among workers at resource material factories.

This study is to assess exposure of bioaerosols and metals from different working areas at a material recovery facility (MRF) in central Taiwan. In order to investigate species, concentrations and size distribution, airborne fungi and bacterial were taken by using an Anderson 6 stage viable impactor and Microbial Air Monitoring System-100 (MAS-100). Airborne dusts were sampled by a ten-stage micro-orifice uniform deposit cascade impactor (MOUDITM), followed analyzed concentrations of Cu, Zn, Cd, Cr, Mn, Ni, Pb and W by inductively coupled plasma optical emission spectrometry (ICP -OES).

In this study, the bioaerosol concentrations did not exceed the standard of occupational exposure limit. Aspergillus was the most predominant fungal isolates, with a mean concentration of 965.3 CFU/m3. Staphylococus warneri was the dominant bacterial isolates identified. Meanwhile, the most prevalent fungi occurred in the size range of 3.3~2.1 µm at recycling of PET bottles area. The most prevalent bacteria were found at recycling of metals area in ≧7.0 µm size range. The major metals in airborne dusts were Zn and Pb， with mean concentrations of 0.71 µg/m3 and 0.64 µg/m3, respectively.

This study indicated that relatively humility was associated with bioaerosol concentrations in MRF environment. Many major indicators of allergenic and toxigenic airborne fungi such as Aspergillus and Staphylococus warneri were found in the material recovery environments. The results obtained from this study may provide useful information for the implementation of management for material recovery facility.

7AE.10

Exposure to Fine Particulate Matter and Black Carbon during Cycling: A Comparison between London and São Paulo.

VERONIKA SASSEN BRAND, Prashant Kumar, Maria de Fatima Andrade, *University of Sao Paulo*

People, during commuting, mainly through active transport, like cycling and walking, are exposed to higher concentrations of traffic emissions due to their proximity to on-road vehicles. Several epidemiological studies relate particulate matter (PM), including the black carbon (BC) fraction, exposure to both mortality and morbidity caused by respiratory and cardiovascular diseases. As a part of ASTRID Project (Accessibility, Social justice and Transport emission Impacts of transit-oriented Development strategies) and PEDALS project (Particles and Black Carbon Exposure to London and Sao Paulo Bike-Lane Users), we did a comparative assessment of commuters exposure to both fine particles ($PM_{2.5}$) and BC in specific cycle routes in the cities of London (UK) and São Paulo (Brazil). In both cities, we measured, during the peak and off-peak hours, $PM_{2.5}$ and BC concentrations using a personal exposure monitoring backpack equipped with a MicroAeth AE51 to monitor BC, a DustTrak II Aerosol Model 8530 monitor in Brazil and a GRIMM EDM 107 aerosol spectrometer in the UK to measure $PM_{2.5}$ concentrations. Three origin-destination (O-D) routes pairs were chosen in both cities. Each O-D pair gave two routes, the first one being along busy/major roads and the second one presumed to be less polluted since we preferably passed through green/blue/quiet areas. Thus, the aim of this work was to: (1) compare the exposure to $PM_{2.5}$ and BC while cycling during peak and off-peak hours at the chosen routes, (2) identify main pollution hotspots resulting in increased exposure, (3) investigate the correlation between the measured concentrations and the type of cycle lane/presence of vegetation/proximity to water bodies, and (4) calculate the inhaled respiratory deposition doses (RDD). We observed that São Paulo had the highest mean concentration of BC (11 µg/m³) and $PM_{2.5}$ (29 µg/m³), while London, in average, showed 5 µg/m³ of BC and 17 µg/m³ of $PM_{2.5}$. $PM_{2.5}$ and BC concentrations were always higher during the morning peak hours when compared to the evening peak hours, except in São Paulo, where the evening peak was the one with the highest mean concentration of BC (11.4 µg/m³). There was also found that cyclists using a route, which passed through the green/open areas and had relatively less traffic volumes, found to be less exposed to both pollutants assessed. The findings in this work are important to policy makers and urban planners when planning new cycle networks with less exposure levels, not only in the two urban areas assessed, but also as a model to other urban locations.

7AM.1

Atmospheric Relevance of Laboratory Experiments on Ion Composition Based on Ion Composition Simulation. KALJU TAMME, Aare Luts, Urmas Hõrrak, Jaan Salm, Heikki Junninen, *University of Tartu*

Composition of small atmospheric ions depends on trace gas composition and concentrations. Atmospheric ions are produced by ionization sources and evolve through a cascade of collisions between ions themselves and neutral trace gas molecules, and are absorbed by recombination, coagulation with particles and diffusion onto walls. Ionization is initialized by collisions of high energy particles from outer space or by radioactive decay.
The main motivation for conducting simulations was to evaluate the effects of temperature, sulfuric acid concentration and absence or presence of CO_2 in reaction on the chemical composition of ions. This study was aimed to give an insight into atmospheric applicability of laboratory experiments that are often conducted in N_2 or synthetic air environment. Among others, those experiments conducted in CERN the Cosmics Leaving Outdoor Droplets (CLOUD) were absent of CO_2. Results from CLOUD showed higher ion concentration and ion-induced nucleation than measured in Hyytiälä, SMEAR station, Finland (Wagner et al, 2015).

The ion-kinetic model introduced by authors was used. Model contained 522 ion-molecule reactions with 166 ion species and 127 neutral compounds. Both, the time variations of the concentrations and the steady state concentrations of individual ion species were calculated. Technically, the time variations were simulated as the time evolutions of individual ion species by way of ion-molecular reactions that started from the primary ions (in this study, 5% O^- and 95% O_2^-). The neutral species were regarded as constants. This assumption was justified because (atmospheric) concentrations of these neutrals were many orders of magnitudes higher than those of ions. The steady state concentrations were computed by the model considering both, the time evolution of the individual ion species and the parameters, that determine the ionization and sink characteristics in a given environment. A more detailed description of the model and some examples where it was used can be found in (Luts and Parts, 2002; Parts and Luts, 2004; Luts and Salm, 1994; Luts, 1994).

We used our model to simulate experiments with absence and presence of CO_2, with different temperatures and different concentrations of H_2SO_4. When compared simulations where the changing parameter was CO_2, we found that in the presence of CO_2 the NO_3^-concentration were still higher than in those made without CO_2. Also in the simulations where CO_2 was present the O_3^- had much lower concentration. As a conclusion we found that CO_2 has an effect on steady-state concentrations of ions. On simulations where the changing parameter was H_2SO_4, we saw that when H_2SO_4 concentration was higher the NO_3^- concentrations were lower. Investigating the behavior of cluster ion composition from temperature, we found that on most simulations NO_2^- and NO_3^- had higher concentrations at higher temperature.

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7AM.2

Comparison of Different Aerosol Dynamics Models Based on Accuracy and Computational Time. GIRISH SHARMA, Sukrant Dhawan, Zhichao Li, David I. A. Dhanraj, Pratim Biswas, *Washington University in St Louis*

Numerical simulation for aerosol dynamics is indispensable tool for predicting the evolution of particulate systems, which is useful for in-depth understanding of the experimental measurements, in atmosphere as well as aerosol reactors. These models permit the interaction of complex physical processes through simulation, which are then related to the experimental data. Different aerosol dynamics phenomena like chemical reaction, nucleation, condensation, coagulation, sintering, aggregate formation, and charging are described using general dynamic equation.

Different numerical schemes have been developed over the years to simulate these processes which include method of moments, discrete model, sectional model, discrete-sectional model, and modal model. Each of these schemes has its own advantages and disadvantages. Among these, discrete representation of particle sizes is the most accurate representation of aerosol dynamics as it mimics the aerosol dynamics most closely, but this comes at a high computational cost whereas sectional model is computationally less intensive but has inaccuracies in small sizes. Method of moments and modal model are very fast but are not as accurate as sectional and discrete models. Although separate literature on all these models exists, the comparison between all the models based on their application under different conditions has not been investigated.

In this work, the aim is to investigate the performance of different aerosol dynamics models under different applications. First, different models will be compared based on the accuracy of their results. Then, these models will be compared based on the computational time required to run a simulation with the same configuration. Finally, the performance of these models will also be analyzed on different computer processors. With the better understanding of the trade-off between accuracy and computational time, a recommendation will be made on choosing aerosol dynamics model for different applications.

7AM.3

Modeling On-road Fine and Ultrafine Particle Concentrations in Los Angeles. Nu Yu, Shi Shu, Lu Zhang, Yan Lin, Jun Wu, YIFANG ZHU, *UCLA*

Air pollution is among the top threats to public health in Los Angeles. Traffic related particulate matter (PM) exposure has been linked to different adverse health effects. In this study, fine PM ($PM_{2.5}$) and ultrafine particle (UFP) concentrations were measured on roadways outside moving taxi vehicles in the Greater Los Angeles area from April to November, 2013. The total distance driven is approximately 11,000 kilometers and the total hours of field measurement is approximately 500 hours. We developed and compared four types of models to estimate UFP and $PM_{2.5}$ concentrations on freeways, arterial roads, and local surface streets: multiple linear regression models without and with temporal variance structures (MLR and sMLR models), and generalized additive models without and with temporal variance structures (GAMs and sGAMs). A backward selection procedure was used to select predictive variables from meteorological condition panel, traffic condition panel, and spatial feature panel. The modeling results show that GAMs explained the highest percentages of the total UFP and $PM_{2.5}$ variance. The MLR models generated the best cross validation (CV) results with least discrepancy from the general R^2s. The models performed the best on the data collected on arterial roads comparing with the data collected on freeways and local streets. The arterial road models generated general R^2s equivalent or above 0.40 and CV R^2s ranging from 0.34 to 0.73. All arterial road models and the local street $PM_{2.5}$ sMLR model and GAM generated both general and CV R^2s greater than 0.30. Temperature, relative humidity, vehicle speed, annual average daily traffic (AADT) and time of day variables were consistently selected by these models. These predictors, except for time of day, show positive associations with UFP or $PM_{2.5}$ concentrations, which are consistent with previous studies, and the physical and chemical properties of the traffic related UFP and $PM_{2.5}$.

7AM.4

Overprediction of Fine Aerosol Nitrate by Chemical Transport Models: The Role of Nighttime Chemistry and Mixing.

Maria Zakoura, SPYROS PANDIS, *University of Patras*

Fine particulate nitrate is often over-predicted by chemical transport models (CTMs) in areas of the Eastern US and Europe. This overprediction is especially severe during a few nights during the summer or other photochemically active periods, when CTMs predict unreasonably high nitric acid production rates. We test the hypothesis that the main reason of this nighttime aerosol nitrate overprediction is the coarse grid resolution used that cannot capture the local phenomena that take place in the plume of major sources. The CTM PMCAMx is used to simulate a summer period over the Eastern US taking advantage of the dense fine nitrate measurement networks (STN and IMPROVE) in that area.

The base case simulation with coarse resolution (36x36 km) often predicted high nighttime nitrate production rates, thus leading to widespread overprediction of aerosol nitrate levels both during the night but also during the next day. We show that this overprediction is due to the artificial mixing by the model of NO_x-rich plumes from major point and area sources with the background atmosphere. The bias for $PM_{2.5}$ nitrate decreased by 65% when the grid resolution was increased to 4x4 km. However, this improvement comes with a significant increase in the computational cost of the simulation.

The ability of a Plume-in-Grid (PiG) approach to increase the accuracy of the model with a small increase in computational cost was also investigated. The PiG sub-model was applied for the gas-phase chemistry only for the major NO_x point sources in the Eastern US during the same period. Different CTM grid resolutions were used. The results suggest that the PiG approach can be a computationally efficient method to reduce the nitrate bias in CTMs.

Despite all the above improvements, systematic discrepancies remain between the model predictions and observations. Other potential improvements in both the simulation of nitric acid partitioning, nighttime chemistry, nitric acid removal, and the emissions of ammonia are discussed.

7AM.6

Regional Climate and Air Quality Impacts of Particulate Emissions from Gasoline Direct-Injection (GDI) Vehicles.

SOROUSH ESMAEILI NEYESTANI, Rawad Saleh, *University of Georgia*

Due to their enhanced fuel economy, the market share of Gasoline Direct-Injection (GDI) engines light-duty vehicles has increased noticeably over the past decade. However, compared to the traditional port-fuel injection (PFI) engines, GDI engines have been shown to emit higher levels of particulate matter, especially black carbon (BC). BC is an efficient absorber of solar radiation, and is a prominent global-warming agent second only to carbon dioxide. This competing effect of reducing carbon dioxide emissions but increasing BC emissions raises a question regarding the net climate impacts of GDI vehicles. Back-of-envelope calculations based on the global-warming potential (GWP) of BC have shown that, on a global scale, switching to GDI vehicles has a net climate benefit of 0.5% – 2.4%[1,2]. However, due to their short lifetime, aerosol climate impacts are more important on the regional scale; therefore, the regional climate impacts of GDI vehicles might diverge from the global impacts in areas where traffic emissions are prominent.

Here, we estimate the regional (over the United States) air quality and climate impacts of switching the U.S. fleet from PFI to GDI vehicles. We use the Weather Research and Forecasting model coupled with chemistry (WRF-Chem), which simulates both chemical transport and radiative transfer. The simulations are performed at a 12 km resolution and for a period of four months (February, May, August, and November) in each season of 2011 to take into account the seasonal variability. Rapid Radiation Transfer Model for GCM (RRTMG) and Modal Aerosol Dynamic for Europe coupled with Secondary Organic Model (MADE-SORGAM) schemes are used in the model for SW/LW atmospheric radiation and aerosol mechanism, respectively. Aerosol Optical Depth (AOD) retrieved from NASA's Aerosol Robotic Network (AERONET) and Moderate Resolution Imaging Spectroradiometer (MODIS) are used to validate model calculations. Using the EPA's National Emission Inventory for 2011 (NEI-2011) as a base case, we modify the vehicle emission profiles using GDI emission data from measurements[1]. By comparing the base case with the modified one, we obtain spatially and seasonally resolved changes in carbonaceous aerosol concentrations and the consequent radiative effect.

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7AM.8

Diffusion Limitations and Shielding Effects in the Ozonolysis of Polycyclic Aromatic Hydrocarbons Embedded in Secondary Organic Aerosols. BRIAN HWANG, Shouming Zhou, Pascale Lakey, Jonathan Abbatt, Manabu Shiraiwa, *University of California, Irvine*

Benzo[a]pyrene (BaP), a key polycyclic aromatic hydrocarbon (PAH), is known as a carcinogen and mutagen. BaP is often associated with soot particles emitted from biomass burning and incomplete combustion. In the atmosphere, BaP can react with oxidants such as ozone forming more toxic compounds including quinones and epoxides. Thus, it is important to quantify the kinetics of the heterogenous reaction between BaP and ozone, which is investigated in this study. The decay kinetics of BaP by ozone were measured by applying direct analysis in real time mass spectrometry (DART-MS) [1]. BaP was embedded in bis(2-ethylhexyl) sebacate or alpha-pinene secondary organic aerosol material. To investigate the impact of phase state on reaction kinetics, experiments were conducted at different relative humidities of < 5%, 50%, and 85%.

We applied the kinetic multi-layer model of aerosol surface and bulk chemistry, (KM-SUB) [2] to model the experiment data. KM-SUB explicitly treats mass transport and chemical reaction at the surface and in the bulk. To obtain the distribution of kinetic parameter values to fit the experiment data with modeling, we applied the Monte-Carlo genetic algorithm method [3]. In this method, kinetic parameters are randomly chosen to fit the experimental data and these values are optimized by genetic algorithm. By considering the decomposition of ozone and subsequent formation of reactive oxygen intermediates [4], the concentration dependence of BaP decay was reproduced using a single set of kinetic parameters. The obstruction theory was applied to account for inhibition of bulk diffusion of the BaP and ozone due to accumulation of reaction products at the surface and in the near-surface bulk [5]. With this approach, we were able to capture the initial fast kinetics followed by slow decay of BaP. We also analyzed how mass transport, rate of surface or bulk reaction, and diffusion of BaP and ozone may limit the overall reaction kinetics, finding that the reactions were controlled by bulk diffusion of BaP from the bulk to the surface at longer reaction times.

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7AM.9

Addition of Charge Model to Coupled Flow-Aerosol Dynamics for Glowing Wire Conditions. KUNAL GHOSH, S.N. Tripathi, Manish Joshi, Y.S. Mayya, Arshad Khan, B.K. Sapra, *IIT Kanpur*

Glowing wires generate charged nanoparticles via electrical heating which have been used earlier in association with mobility classification, but the phenomenon is complex and not fully understood. C. Peineke, A. Schmidt-Ott[1] explained generation of negative particle charge by thermoemission of electrons and positive particle charge by surface ionization of impurity atoms with low ionization energy. Such impurities are inevitably present even in high-purity metals. The role of charge, for such conditions, via coupled flow aerosol dynamical equation has not been studied. Our previous work discusses CFD coupled aerosol microphysics model (without charge) in context of aerosol generation from a glowing wire. In the present work, we have added particle charge to aerosol dynamics sub-modules (ion-induced nucleation, charged particle coagulation[2], electrostatic dispersion[2]) along with Navier Stokes equations. The model is also suitably modified to include buoyancy coupled K-Epsilon turbulence scheme. Coupled flow-aerosol dynamics equation was solved numerically and in implicit scheme. Wire composition and temperature (wire surface and cell domain) were obtained/measured, to be used as input for the model simulations. The aerosol dynamics scheme has been tested for charged aerosol particles by model studies against published results and the complete model was validated against measured temporal evolution of total number concentration and size distribution at the outlet of hot wire generator cell.

Model simulations showed significant effect of fluid properties and charge on aerosol dynamics if charge level is higher than the Boltzmann equilibrium charge limit for less than 1 µm particles. Experimental results have been compared with model simulations made for unipolar as well as bipolar charge distribution function. Although tuned specifically for the present context (i.e. aerosol generation from hot wire generator), the model can also be used for diverse applications e.g. emission of particles from hot zones (chimneys, exhaust), fires and atmospheric cloud dynamics.

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7AM.10

Aerosol Nucleation Activated by Inducing Factors in Coal-Fired Flue Gas: A Simulation Study. CHENGSI LIANG, Chenghang Zheng, Zhengda Yang, Yi Wang, Weiguo Weng, Xiang Gao, *Zhejiang University, China*

Aerosol nucleation is an important process in the formation of aerosols in flue gas from coal-fired power plants. Ultrafine particles will form in desulfurization tower because of the huge drop in temperature, which is hard to be removed and may pollute the environment. Molecule dynamics (MD) is an approaching way to study the nucleation without the huge calculated amount to get the force between different kinds of molecules and clusters. Based on the fact that the number of water molecules is much more than other kinds of molecules in the unit volume flue gas, the model of cluster, which contains one inducing molecule in the center, like a sulfuric acid molecule or charged molecule, and multilayer water molecules around it, was established. The distribution of water molecules around the center molecule were acquired by calculating the structure of clusters with different numbers of water molecules. And the force field around the cluster was acquired by calculating the change of free energy when one more water molecule move towards to the cluster. All of the above calculations were realized through the density functional theory (DFT) method. It found that, comparing to pure water vapor nucleation, the extra effects from the center molecule to the water molecules which are in the same water molecules layer are similar, and the extra effect decreases along when the layer increases until it can be ignored. Therefore, the influence of the center molecule on finite layers of water molecules was considered to simplifying the model. This simplified cluster model was used to investigate nucleation process in dynamical method. This work figured out the nucleation rate and dew point of aerosol in different conditions, which basically correspond to the acid dew point by measurement.

7AM.11

Carbon-, Oxygen-, and Size- Resolved Model to Simulate the Microphysics, Chemistry, and Thermodynamics of Biomass Burning Organic Aerosol. ALI AKHERATI, Christopher Cappa, Jeffrey R. Pierce, Shantanu Jathar, *Colorado State University*

Globally, biomass burning – that includes wildfires, agricultural, prescribed and landfill burning – is an important source of organic aerosol (OA) to the atmosphere. Emissions of biomass burning organic aerosol (BBOA) vary substantially with the fuel type, burn conditions, and ambient conditions and atmospheric mixing and photochemical oxidation are expected to alter the size, mass, and composition of BBOA. Yet, there are large uncertainties when it comes to understanding the physicochemical evolution of BBOA and its consequent impacts on air quality, climate, and human health.

In this work, we will develop a state-of-the-science OA model that combines the two-dimensional statistical oxidation model (SOM) with the TwO-Moment Aerosol Sectional (TOMAS) model.The SOM uses a two-dimensional carbon-oxygen grid to track the gas- and particle-phase chemistry, gas/particle partitioning, and properties of gas- and particle-phase organic precursors and products. The TOMAS model uses two moments, that of number and mass, of the aerosol size distribution to model processes of nucleation, condensation, and coagulation. This updated model, resolved in dimensions of carbon number, oxygen number, and size, will simulate the microphysics, chemistry, and thermodynamics of BBOA and include the following processes: (a) semi-volatile and reactive POA, (b) SOA formation from semi-volatile, intermediate-volatility and volatile organic compounds, (c) multi-phase, multi-generational aging that includes functionalization and fragmentation reactions, (d) low-volatility SOA formation from autoxidation and oligomerization reactions, (e) influence of vapor wall losses encountered in laboratory SOA formation experiments, and (f) phase state of OA. The model will be evaluated against chamber and flow reactor experiments performed at the Fire Laboratory in Missoula, MT as part of the FLAME and FIREX campaigns to identify the most important precursors, pathways, and experimental artifacts that control the size, mass, and composition of BBOA.

Insight from this work will be used to develop models and parameterizations for BBOA in regional and global air quality and climate models.

7AM.12

Estimation of Loss Rates from Chamber Experiment Data Using a Statistical Inverse Approach. MATTHEW OZON, Aku Seppänen, Ari Leskinen, Jari Kaipio, Kari Lehtinen, *University of Eastern Finland*

Motivations

Deposition is one of the key aerosol microphysical processes, important in large scale when considering both climate and health effects and in a smaller scale, e.g. when analyzing chamber experiments. Deposition mechanisms and rates are strong functions of size: smaller particles deposit mainly by diffusion in contrast to larger ones, which deposit by settling or due to their inertia. In this study, our focus is on estimating deposition rates in experiments, e.g. in a chamber, in which multiple processes are acting simultaneously. One might for example encounter a situation in which the concentration is high enough that coagulation is significant in addition to deposition. Then it is not straightforward to extract size dependent deposition rates just by simply examining the decrease of the number distribution.

Methods

A rigorous method to estimate size dependent deposition rates in a chamber has been to perform several separate concentration decay experiments using a monodisperse aerosol. This is, however, not necessary even for a seemingly complex case with other simultaneous disturbing processes if advanced data-analysis methods are used. Here we propose an automated method where the only assumption is that the parameters vary “slowly” over time. Our approach relies on the widely used statistical, dynamical inversion method that accounts for measurement uncertainty in a rigorous way, the Kalman Filter (KF). The KF is stable, minimizes the variance of the estimates and is easy to implement. Our implementation of the KF not only filters — improve the data quality — the size distribution, but it also estimates the global loss rates. Most importantly, this method only relies on a physical evolution model — the aerosol General Dynamic Equation — a measurement model —SMPS— and rough uncertainty estimations that are combined in the KF framework.

Results

As a proof of concept of our method we analyze synthetic data generated by solving the GDE with an accurate sectional method. The data are simulated using a time invariant, arbitrary loss rate and a size spectrum ranging from an arbitrary critical cluster size of 2nm to 2µm. In this simulation, there is no vapor present, and thus the particles do not grow by condensation and there is also no nucleation. Additionally, the data are corrupted by additive and multiplicative noise in order to resemble actual measured data. The results show that the global loss rates are well estimated. Finally, the method is applied to SMPS data from a real wall loss experiment. The estimated parameters are of the same order of magnitude as those previously manually computed, and the size dependence is similar to what is expected by the theory.

7AM.13

The Effect of Fiber Polydispersity on Filtration Modeling. SEUNGKOO KANG, Da-Ren Chen, David Y. H. Pui, *University of Minnesota*

Fibrous filters are widely used to remove aerosol particles. To design a filter with desirable filter structures and properties, estimation of filtration performance of fibrous filter media is essential. A majority of studies have modeled computational filter domains with uniform-sized fibers, i.e. the domain is composed of monodisperse fibers, while real fibrous filter media are composed of polydisperse fibers. In this study, a filtration domain composed of randomly distributed polydisperse fibers is presented with its properties, such as the thickness and solidity, the same as the real filter media. In the modeling, the collection efficiencies of filters were obtained from the numerical model using particles in the size range from 3 to 500 nm, and these efficiencies were compared to the efficiencies from experimental data. In addition, the collection efficiencies from computational domains with uniform-sized fibers were also compared in order to investigate the effect of fiber polydispersity. It was found that collection efficiencies are significantly affected for the domain with monodisperse fibers depending on the fiber size and filter types, while the domain with polydisperse fibers showed an excellent estimation of efficiencies regardless of filter types. Via the validated model, we also examined the effect of fiber polydispersity on the collection efficiency for domains having the same arithmetic mean fiber diameter and properties such as solidity and thickness. Results showed that the particle collection in filter media is affected by the degrees of fiber polydispersity, especially for particles in the size range between 10 and 100 nm. For fibrous filters having bimodal size distributions, the collection efficiency was influenced by the degrees of fiber polydispersity and the size and volume fraction in each fiber mode.

7AM.14

Sensitivity of Sulfate In-cloud Chemistry and CCN Activation to pH Variability and Mixing State Using a Particle Resolved Model. YU YAO, Nicole Riemer, Matt Dawson, *University of Illinois at Urbana-Champaign*

Over 50 percent of the total sulfate mass at the global scale is produced by in-cloud aqueous phase chemistry that oxidize S(IV) to S(VI), and the reactions can change the particle size distribution after cloud evaporation. It is well known that different reaction pathways contribute to these oxidation processes, and that the relative importance of the pathways depends on pH. However, for current regional and global scale models it is challenging to capture the effects of non-linearity in reaction rates that may occur due to differences in droplet composition in the highly externally mixed aerosol systems often found in the real atmosphere.

In this study, we focus on the sensitivity of sulfate formation to aerosol mixing state and related variations in pH across the particle population. We simulated several urban plume scenarios that produced populations with a wide range of different aerosol mixing states using the particle-resolved model PartMC-MOSAIC. These simulated aerosol populations were then used as the input for cloud parcel simulations including aqueous chemistry where we found the sulfuric species transition mainly between sulfate, bisulfite and hydrogen sulfate under different pH and oxidation environments. The aqueous chemistry mechanism coupled in the model is based on a reduced version of CAPRAM 2.4 developed by Ervens et al. in 2003, which includes 121 aerosol species and 178 reactions. The particle-resolved approach is well-suited for this problem because it can track the evolution of compositions in each particle, including the concentration of H+. We quantified how sulfate formation changes the CCN properties of the aerosol population after cloud evaporation and how this depends on the mixing state of the cloud-forming aerosol. The results will also be used to quantify the uncertainties of CCN properties due to the assumptions of the aerosol mixing state.

7AM.15

Quantifying Errors in CCN Concentration and Aerosol Optical Properties Caused by a Non-Interactive Coarse Mode Using a Particle-Resolved Aerosol Model. JESSICA GASPARIK, Nicole Riemer, Jeffrey H. Curtis, *University of Illinois at Urbana-Champaign*

Coarse mode aerosols are generally considered to be particles of primary origins (e.g., dust, sea salt, pollen, small pieces of rubber from automobile tires) with diameters greater than ~2 µm. They are emitted into the atmosphere through mechanical processes and have a lifetime on the order of hours to days. Although this is a relatively short lifetime, many coarse mode particles still have sufficient opportunities to interact with finer mode aerosol particles (including Aitken, and accumulation modes) by coagulation, or provide surface area where secondary aerosol material can condense on, causing changes in the distribution of aerosol number mass. However, in many global models the coarse mode is treated as non-interactive, meaning they do not consider coagulation of coarse mode particles with the rest of the distribution and interaction with the gas phase. While this reduces computational cost, it may introduce significant error in predictions of the size distribution, cloud condensation nuclei (CCN) concentrations, and aerosol optical properties. The objective of this study is to assess the interactions between the coarse mode with other particle size ranges and determine the conditions where it is acceptable to treat the coarse mode as non-interactive.

For this study, we used a particle resolved model, PartMC-MOSAIC coupled with the WRF model. The model resolves the aerosol composition on a per-particle level in a Eulerian single-column domain and couples the aerosol and gas-phase chemistry with the meteorology. We constructed a suite of scenarios representative of a large urban area and simulated the evolution of aerosols of different emission types due to coagulation, condensation of secondary aerosol, and vertical mixing within the column. We varied the emissions of coarse mode and finer modes, particularly from combustion sources along with the vertical mixing by turbulent diffusion within the column. In each scenario, we compared the aerosol properties when the coarse mode is treated as interactive versus non-interactive, with respect to time and height. Based on this error, we identified conditions when it is acceptable to consider the coarse mode as non-interactive.

7AM.16

Soil NOx Emissions and Particulate Nitrate Formation in California. Abhishek Dhiman, Anikender Kumar, Maya Almaraz, Ian Faloona, Benjamin Houlton, MICHAEL KLEEMAN, *University of California, Davis*

PM2.5 concentrations in California continue to violate the National Ambient Air Quality Standards designed to protect human health. The highest PM2.5 concentrations occur during winter months with major contributions from particulate ammonium nitrate. Chemical transport models are used to help design efficient emissions control programs to address PM2.5 pollution, but these models have generally failed to predict basecase particulate ammonium nitrate concentrations in recent years. This calls into question the accuracy of future emissions control strategies for PM2.5 in California.

Recent work suggests that soils enriched with nitrogen fertilizers release oxides of nitrogen (NOx) that can play a role in atmospheric chemistry. Here we analyze the effect of soil NOx emissions on winter particulate nitrate formation and summer ozone formation in California. Monthly emissions of soil NOx are estimated based on fertilizer application rates, soil types, soil moisture, and temperature. These emissions are combined with standard emissions inventories provided by the California Air Resources Board. Episodes spanning the years 2000 through 2016 are simulated with and without soil NOx emissions using a regional chemical transport model. Predicted concentrations are compared to measurements to quantify improvements to model performance. Source apportionment routines are used to predict soil NOx contributions to ambient PM2.5 concentrations. Public health impacts are quantified using established epidemiological findings to estimate the potential health effects of soil NOx emissions in California.

7AM.17

Characterization of an Ultra-low Flow-rate Hydrocyclone. HYUNWOO LEE, Youngjin Seo, *Kumoh national institute of technology*

Hydrocyclone is a device for separating particles by centrifugal force from water which is a working fluid. Because of its advantages such as real-time separation and no moving part in it, it is used in numerous applications such as classifying, solids separation and concentration, etc. The objective of this study is to numerically characterize the particle separation efficiency by changing the design of hydrocyclone that operates at flow-rate of 1 LPM. To do so, we changed the diameter of the vortex finder and the length of the conical section, etc. The specific gravity of the injected particles is 1.25. The numerical analysis results showed that 5 µm particles or larger could be separated 100%. In addition, separation efficiency became enhanced when the design of hydrocyclone was changed. For instance, the efficiency was improved as the diameter of the vortex finder was decreased, but the flow rate of the purified working fluid was decreased. We will also present experimental data using the optimized hydrocyclone.

7AM.18

Modeling the Dynamics of Fractal-Like Soot Aggregates Using the Specialized Aerosol Solver. VICTOR GRYAZIN, Sergey Beresnev, *Ural Federal University, Ekaterinburg, Russia*

Various applications of processes of radiation absorption and motion of soot particles are well-known under the numerous publications. Among them appreciable interest is caused by experimental and theoretical researches of the radiometric phenomena (thermo- and photophoresis) with carbonaceous aerosols well absorbing radiation practically in the all range of radiation wavelengths. Such investigations require numerous calculations; therefore specialized aerosol solver for a wide range of calculations related to the photophoretic motion of soot particles is developed. It is useful to keep the mathematical formalism used in model of homogeneous spheres (the general solution of fractal-like particle problem is extremely difficult).

The calculation of force and velocity of longitudinal radiometric photophoresis is based on the molecular-kinetic theory of this phenomenon (Beresnev et al, 1993). For calculations of optical characteristics for fractal-like particles it is possible to use methods of effective medium approximations (e.g., Chylek et al, 1988) and theoretical predictions for fractal-like soot particles by Mackowski (2006). It was revealed that the choice $m = 1.764+0.570i$ for $\lambda = 0.68$ µm (the wavelength of the He-Ne laser) is optimum. Effective thermal conductivity of fractal-like soot particles can be calculated using the method offered for estimation of thermal properties of nanofluids with significantly enhanced thermal conductivity by the aggregation of nanoparticles into clusters (Evans et al, 2008).

The determined above characteristics are used in gas-kinetic calculations for photophoretic force and velocity. Reliability and accuracy of suggested model is necessary to estimate by comparison with adequate experimental and theoretical data. The experimental results of Karasev et al (2004) on photophoretic velocities of soot particles in nitrogen provide a unique opportunity to compare results. In experiment two groups of aggregates sizes distinctly differ: small particles at $R_m \leq 0.5$ µm and large particles $R_m > 0.5$ µm for which the mobility radius R_m was defined by various techniques at invariable fractal dimension $D_f = 1.80$.

It is obvious, that for the quantitative description of fractal-like aggregates photophoresis it is necessary to have a strict theoretical method for prediction of parameter Λ on the basis of knowledge of fractal dimension of the aggregate D_f and thermal characteristics of primary particles.

The analysis has shown that for a qualitative and quantitative explanation of photophoretic motion of aggregates it is possible to apply the well-developed theory for homogeneous spherical particles at correct treatment of key parameters.

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7AM.19

Regional-scale Impacts of Primary Ultrafine Particle Emissions in the United States. BENJAMIN MURPHY, Francis Binkowski, Ekbordin Winijkul, Matthew Alvarado, *United States Environmental Protection Agency*

Direct particle emissions substantially increase ultrafine particle (UFP) concentrations near emission sources and have impacts on aerosol properties like bulk surface area. However, standard emission inventories like the National Emission Inventory (NEI) report only bulk coarse and fine particle mass emission factors and so most chemical transport models do not explicitly account for the impacts of the large magnitude of UFP number emissions. This gap has important implications for understanding and managing air quality in the U.S. with respect to particulate pollution.

We have updated the Community Multiscale Air Quality (CMAQ) model with new algorithms and data to investigate the contributions of specific emissions sectors to UFP concentrations throughout the US. This research version of the model, called CMAQ-UFP, includes improved parameterizations of aerosol emissions from a single-distribution approach to a rich dataset of multiple distributions with dependencies on emission source, technology, and fuel. The new model gives a more complete representation of the complexity of UFP sources, sinks, and potential impacts.

We apply the new model to specific observations made throughout the U.S. including California and the mountain west. This combination of sites allows us to evaluate the model against detailed in situ and remotely-sensed particle properties. It further allows us to characterize the model in urban/suburban regimes with dramatically varying contributions from individual sources. Finally, we use this platform to quantify the spatio-temporal variation in the contribution of primary/secondary sources to particle number and surface area, two metrics thought to be important for connecting particulate pollution to human health impacts. This exercise improves our understanding of the most effective ways to mitigate the highest UFP concentrations in the US.

7AM.20

Developing the SAPRC Gas-Phase Chemical Mechanism and Chamber-Based SOA Parameterizations for Evaluating Biomass-Burning Derived SOA from Furan and Furan Derivatives. JIA JIANG, William P. L. Carter, David R. Cocker III, Lindsay Hatch, Kelley Barsanti, *University of California, Riverside*

Biomass burning (BB) can release significant quantities of trace gases and particulate matter (PM) to the atmosphere, which will strongly influence climate and tropospheric air quality. Advances in analytical techniques have recently enabled improved identification and quantification of the gas-phase organic carbon emissions from BB. Efforts to quantify the potential secondary organic aerosol (SOA) formation from these recently identified compounds have been hindered due to the lack of published information on the reaction kinetics and mechanisms for atmospheric oxidation, as well as the lack of chamber-based SOA yields. Furan and its derivatives represent one significant class of compounds in BB emissions, for which the fate and potential role as SOA precursors remain largely unexplored.

Here we present recent developments in: 1) the SAPRC gas-phase chemical mechanism to treat the atmospheric oxidation of furan/furan derivatives; and 2) SOA parameterizations for furan/furan derivatives derived from existing chamber data. Prior to this study, the treatment of furan chemistry in SAPRC was highly condensed and parameterized, which made it less reliable for atmospheric predictions in BB-influenced regions. Reaction rates of furan/furan derivatives with atmospheric oxidants and subsequent product yields were updated based on published literature specific to furan/furan derivatives and structure-activity relationships; the mechanism, including recent updates, was designed to be applicable for both low and high NOx conditions. Smog chamber data from fifteen experiments with furan or its methyl derivatives were used to evaluate the SAPRC model with updated furan/furan derivative chemistry. Additionally, SOA parameterizations were derived by fitting measured SOA yields (wall-loss corrected) using a Volatility Basis Set (VBS) modeling approach. The updated gas phase and SOA modeling results will be presented. Together the updated SAPRC mechanism and chamber-based SOA parameterizations will allow predictions of the potential contribution of BB-derived furan and furan derivatives to SOA formation using chemical transport models. Future work will include additional chamber studies to investigate a wider range of furan derivatives and chemical conditions most relevant in fire-impacted regions. Modifications to the SOA parameterizations to better represent the range of formation processes will also be considered.

7AP.21

Evaluation and Comparison of Aerosol Properties at Two Background Sites in the Central Amazon Rainforest. MARCO AURÉLIO FRANCO, Luciana Rizzo, Paulo Artaxo, *University of São Paulo*

The Amazon rainforest is the largest tropical forest in the world and occupies approximately half of the Brazilian territory. Its huge ecosystem interacts directly with the atmosphere, making the forest a biogeochemical reactor with capacity of regulation of climatic processes on a continental scale. The Amazon is one of the few continental regions of the Earth where the atmosphere in the rainy season is considered in pristine conditions, allowing for detailed studies of natural processes that controls generation and influence of aerosols on climate. In particular two sites, ATTO and ZF2, are of great relevance in the study of background aerosols properties in the Central Amazon, both sites located upwind the pollution plume of the Manaus city. The ATTO and ZF2 sites are located 160 and 60 km from the city, respectively, both surrounded by undisturbed forests. Due to the proximity, it is possible that the ZF2 is occasionally affected by the Manaus plume.

In this study it was evaluated the distribution of natural aerosols at the ZF2 and ATTO sites based on their physico-chemical properties. The data used in this analyzes were taken simultaneously at the sites between 2014 and 2016 , including particle light scattering and absorption coefficients, number concentration, number size distribution and chemical composition with nephelometer, MultiAngle Absorption Photometry, Scanning Mobility Particle Sizer and Aerosol Chemical Speciation Monitor. The analysis showed that both in dry and rainy seasons the aerosol scattering coefficients at 525 nm has differences between the sites. In the dry season of 2014 there were two events, probably regional fires, one in August and another in September, in which the scattering coefficient reached values greater than 200 Mm^{-1} at the ZF2 site and 140 Mm^{-1} at the ATTO site, respectively. Analyzes of the single scattering albedo (SSA) in 637 nm using boxplots showed that the median value in August at the ATTO site was 0.81 and at the ZF2 site the median was 0.91.

In September, the median SSA in the ATTO site was 0.83, while at the ZF2 site the median SSA was 0.87, what indicate predominance of more light scattering particles in ZF2 site in comparison of those at the ATTO site. In the rainy season of 2014, other two aerosol events occurred in March and April, raised the scattering coefficient to approximately 60 Mm^{-1} at the ATTO site, while at the ZF2 site its values remained at approximately 40 Mm^{-1}.Analyzes of SSA in these months showed that in the ATTO site the median was 0.93 for both March and April, while in the ZF2 site the median was 0.81, showing predominance of light absorbing particles at the ZF2 site. Monthly boxplots for SSA showed opposite behaviors at both sites. While in the ZF2 the monthly median of SSA increases between January and August and decreases between October and December, in the ATTO there are very clear oscillations, with values of medians higher in the rainy season and lower in the dry season, with predominance of more light scattering particles at this site. Those results indicate unexpected inhomogeneity in the optical properties of the aerosols between both sites, and can be caused by the presence of different types of particles in both sites, probably by pollutants from Manaus that reach ZF2 site.

7AP.22

Mass Accommodation and the Condensation Rate for Nanoclusters. Huan Yang, Eirini Goudeli, CHRISTOPHER HOGAN JR., *University of Minnesota*

In modeling particle growth in the gas phase, the condensation rate for nanoparticles is most commonly calculated with a hard-sphere derived equation, in which the condensation rate coefficient scales with the square root of the temperature (i.e. the free molecular condensation rate equation). However, molecular scale clustering reactions, in which two vapor molecules/atoms collide and bind to one another to form a condensed phase entity, often have rates which decrease with increasing temperature. As condensational growth proceeds from the molecular scale to the particle scale, the condensation rate coefficient therefore must undergo a shift from molecular scale behavior (decreasing with temperature) to particle scale behavior (increasing with temperature). Using molecular dynamics trajectory calculations combined with classical collision rate theory, we have examined the evolution of the condensation rate coefficient and the degree of mass accommodation (binding efficiency) for homogeneous condensation onto gold and magnesium nanoclusters (composed of 6-50 atoms). Interestingly we find that for each cluster, above a critical temperature, there is a transition in the condensation rate coefficient; below the critical temperature its derivative is positive with temperature, and above it its derivative with respect to temperature can become negative. Critical temperatures, particularly for the smallest clusters, are found to be well below the melting temperature of the cluster, and at the critical temperature clusters are still stable over the time scales of simulations. We additionally examine high speed atom-nanocluster collisions, which do not lead to binding/condensation, but instead lead to cluster dissociation.

7AP.23

Exploring the Room Temperature Sensing Mechanism of SnO2 Nano-Columns Synthesized by Aerosol Routes towards Volatile Organic Compounds: Theoretical Calculations Compared to Experimental Results. AHMED A. ABOKIFA, Kelsey Haddad, John Fortner, Pratim Biswas, *Washington University in St Louis*

SnO_2 is a wide bandgap semiconducting metal oxide that has been broadly employed as the active sensing material in chemiresitive gas sensors. Recent studies demonstrated the capability of bare-SnO_2 sensors to detect various gases, including volatile organic compounds (VOCs), at room temperature. To explore the sensing mechanism, the adsorption of ethanol and acetone on the (110) and (101) surface facets of rutile SnO_2 is investigated via density functional theory (DFT) calculations and *ab-initio* molecular dynamics (AIMD) simulations. The role of surface oxygen defects, polarity of the VOC molecule, and pre-adsorbed oxygen species from the ambient atmosphere is explored. Theoretical calculations are supplemented by sensing measurements for ethanol using SnO_2 nanostructured thin film sensors fabricated by an aerosol chemical vapor deposition (ACVD) technique.

DFT results show that the direct adsorption of both ethanol and acetone on the (110) and the (101) surface facets of SnO_2 is energetically favorable. The adsorption of both molecules is accompanied by the release of charge from the adsorbate gas to the surface, which promotes the sensing response. Binding strength of both molecules on the stoichiometric (110) and (101) surfaces is greater than that on the oxygen defective surfaces. Ethanol adsorption is generally stronger than acetone due to the bipolar nature of the hydroxyl (OH) group that interacts with the surface via two distinct charge transfer modes. To date, the most cited model regarding the sensing mechanism of metal oxide chemiresistive sensors is through the interaction with the ionosorbed (O^-) species that possess high activity towards oxidizing target gas molecules. However, at room temperature, the less active superoxide molecules (O_2^-) constitute the majority of the pre-adsorbed oxygen species on the SnO_2 surface. DFT results show that minimal interaction takes place between the pre-adsorbed oxygen species (O_2^-) and the studied polar VOCs upon their adsorption on the reduced surfaces. Taken together, these results suggest that the sensing mechanism of SnO_2 towards polar VOCs at room temperature can be explained by their direct adsorption on the surface rather than through their oxidation by means of ionosorbed oxygen species.

7AP.24

Nucleation and Growth of Iodic Particles in the CERN CLOUD Experiment. XUCHENG HE, Lubna Dada, Siddharth Iyer, Hanna Manninen, Yee Jun Tham, Joao Almeida, Dexian Chen, Dominik Stolzenburg, Changhyuk Kim, Arttu Ylisirniö, Maija Peltola, Theodore Koenig, Henning Finkenzeller, Mario Simon, Andrea Baccarini, Richard Flagan, Neil Donahue, Siegfried Schobesberger, Katrianne Lehtipalo, Rainer Volkamer, Douglas Worsnop, Matti Rissanen, Markku Kulmala, Jasper Kirkby, Mikko Sipilä, *University of Helsinki*

Trace iodic vapours have a significant impact on atmospheric chemistry, influencing catalytic ozone destruction and the HOx and NOx cycles. Oxidised iodine species also form aerosols in coastal and polar regions [1], so they play a direct role in Earth's radiation balance. It was recently shown that iodic acid (HIO_3) forms new particles in coastal and polar regions [2] but the chemical pathways leading to HIO_3, and the nucleation and growth rates of iodic particles, remain poorly understood.

In a comprehensive series of experiments performed under atmospheric conditions in the CLOUD chamber [3] at CERN, we have investigated how the precursor vapours iodine and diiodomethane are oxidized to HIO_3; we have also measured the resulting nucleation and growth rates of iodic particles. Surprisingly, we found that HIO_3 forms over a range of relative humidity via a previously-unknown mechanism. We have combined our laboratory experiments with quantum chemical calculations to resolve the exact chemical steps leading to the formation of HIO_3 in the atmosphere.

A bromide chemical ionization time of flight mass spectrometer was used to measure the concentration of molecular iodine at atmospheric concentrations while simultaneously measuring iodic acids and oxides for the first time. This instrument enabled us to comprehensively track the role of individual iodine species in the gas-phase chemistry and nucleation processes.

We have measured the nucleation and growth rates of pure iodic particles. By comparing experiments under neutral (ion-free) and GCR (galactic cosmic ray) conditions [3], we find an important contribution of ions to the nucleation and initial growth rates. Using a suite of state-of-the-art high-resolution instruments, we were able to follow the appearance and growth of iodic particles from an HIO_3 dimer to sizes above 10nm, with chemical identification throughout the entire size range. The data reveal that several growth mechanisms are involved, depending on the particle size.

Our laboratory findings should help to interpret observations of new particle formation in coastal and other regions in the presence of gas-phase iodic species. And the results indicate there are unrevealed oxidation pathways that can affect the fate of ozone in the atmosphere.

[1] O'Dowd, C. D. et al. (2002). Marine aerosol formation from biogenic iodine emissions. Nature 417.

[2] Sipilä et al. (2016). Molecular-scale evidence of aerosol particle formation via sequential addition of HIO3. Nature 537.

[3] Kirkby et al. (2011). Role of sulphuric acid, ammonia and galactic cosmic rays in atmospheric aerosol nucleation. Nature 533.

7AP.26

Simulations of Light Scattering from Aligned and Randomly Oriented Polydisperse Aggregates for Determining Aggregate Shape.

GEORGE MULHOLLAND, James Corson, Michael Zachariah, *University of Maryland*

This study focuses on the simulation of the light scattered by aligned and randomly oriented fractal aggregates of touching spheres. We find from the simulations that a shape parameter for a population of aggregates can be determined from these scattering calculations. The dependence of the structure factor, *S*, on the magnitude of the scattering wave vector, *q*, has been an important tool in the study of the size, the fractal dimension, and the pair distribution function for randomly oriented aggregates. However, such measurements do not provide a measurement of the shape of the aggregate. As discussed in a previous paper (Mulholland, G.W. et al., 2013), an aggregate aligned by an electric field in the direction of the largest principal radii of gyration will scatter more intensely in the forward direction than in other orientations because there is less destructive interference. The scattering plane is oriented perpendicular to the electric field. This paper also showed that a ratio of slopes computed from small angle light scattering intensities is related to the shape parameter A_{31}, which is the ratio of the largest to the smallest principle radii of gyration of the inertia tensor. This measure of shape anisotropy may be an important property regarding the transport of the aggregates, the aggregation rate, the collection efficiency by a filter, and for the characteristics of manufactured aggregates. Since A_{31} is unity for a sphere, a measurement of A_{31} can also be a sensitive diagnostic for the presence of aggregates in an aerosol such as an atmospheric cloud.

In the present study, aggregates were generated to simulate the range of aggregate sizes (30 to 2000), primary sphere radii (10 nm – 23 nm), and size distributions for soot from buoyant turbulent flames at long residence times for a range of hydrocarbon fuels(Koylu, U.O.et al., 1992). More nearly monodisperse aggregates were also generated to simulate the size distributions obtained via mobility or mass classification. The aggregates were generated for a fractal dimension characteristic of classical diffusion–limited cluster-cluster aggregation (DLCA) using an algorithm developed by Mackowski (2006). The value of $S(q)$ was computed for the aligned (but free to rotate about the alignment axis) and randomly oriented clusters. The aggregates were aligned by the electric field in the direction yielding the minimum energy associated with the polarizability of the aggregate. This direction was computed using an algorithm developed by Mansfield et al. (2001).

Results on the correlation between the ratio $\{S(q)\}_a / \{S(q)\}_r$ for the monodisperse and polydisperse clusters and the average value of A_{31} indicate that light scattering measurements in the q range of fractal behavior would be feasible for shape characterization. Also for small q (Guinier regime), the strong correlation between A_{31} and the ratio of slopes of $S(q)^{-1}$ vs. q^2 previously obtained for single aggregate simulations is also valid for polydisperse aggregates. This suggests that small angle light scattering measurements would provide shape information.

The fundamental differences in the light scattering and the pair correlation function for the aligned and randomly oriented clusters will also be discussed.

7AP.27

Spreading Ratios for Aqueous to Glassy Aerosol Particles Using Atomic Force Microscopy (AFM). ZIYING LEI, Nicole Olson, Rebecca Craig, Andrew Ault, *University of Michigan*

The viscosity of atmospheric aerosol particles is a fundamental property that impacts heterogeneous chemistry, phase transitions, and hygroscopicity. Viscosity can be related to the spreading ratio of impacted particles through viscoelastic properties. Particle size, chemical composition, and relative humidity (RH) all affect viscosity, and need to be accounted for when determining and predicting aerosol particle spreading ratios after impaction. However, the viscosity of atmospheric particles is currently poorly quantified, and understanding of spreading ratios from aqueous to glassy aerosol particles is still incomplete. This study aims to determine the relationship between spreading ratio and viscosity of standard aerosol particles composed of inorganic and organic standards. To determine spreading ratio as a function of particle size and RH, laboratory experiments were conducted on size-selected particles (50 – 1,000 nm) under a range of RH conditions (10 – 90%). Atomic force microscopy (AFM) was used to characterize the morphology, height, and projected area diameter of particles, from which the spreading ratio was calculated for individual particles. Changes in spreading ratios were observed with increasing aerosol particle size, as well as with decreasing RH. A fundamental understanding of spreading ratios is will provide insight into the viscosity of aqueous to glassy aerosol particles, which has important implications for water uptake and heterogeneous reactivity.

7AP.28

Characterizing Mass-resolved Mixing State of Black Carbon in Beijing Using Morphology-Independent Measurement Method. CHENJIE YU, Dantong Liu, Kurtis Broda, Rutambhara Joshi, Jason S. Olfert, Hugh Coe, James Allan, *University of Manchester*

The mixing state of black carbon (BC) significantly determines its absorbing efficiency and may modify its regional and global radiative forcing impact and may also influence toxicology. Here, with the aim of identifying the mixing state of BC, an experiment was devised as part of a large joint UK-China project investigating air quality in Beijing, Air Pollution and Human Health-Beijing (APHH-Beijing). During this experiment, we successfully applied a morphology-independent mass measurement of BC for intensive measurements in both winter and summer. We directly selected the particle mass using a Centrifugal Particle Mass Analyser (CPMA, Cambustion Ltd) and passed these monodisperse particles to a single particle soot photometer (SP2, DMT inc.) to characterize refractory BC mass for each single BC-containing particle. The coupling of CPMA-SP2 can thus quantify the mixing state of BC without assuming any particle morphology. The CPMA-SP2 results have been applied to a recently published inversion algorithm to derive the full distributions of particle number according to total mass and rBC mass. Such detailed mass-resolved BC mixing information could be used as optical model input to estimate the optical properties, and also the micro-scale processing model to investigate the atmospheric processing of BC.

7AP.29

New Insight Into Arctic Atmospheric Aerosol Formation. LISA BECK, Clemence Rose, Ella-Maria Duplissy, Matthieu Riva, Federico Bianchi, Olga Garmash, Heikki Junninen, Clara Hoppe, Alexander Schulz, Viola Angelo, Vitto Vitale, Mauro Mazzola, David Cappelletti, Markku Kulmala, Veli-Matti Kerminen, Mikko Sipilä, *University of Helsinki*

Particle formation is globally contributing approximately 50% of cloud condensation nuclei. With increasing temperature, the emission of gases from the different spheres, like hydrosphere, biosphere but also the fauna, is changing; consequently, the molecular composition of the atmosphere is changing. To understand the extent to which the temperature rise and sea ice loss may contribute to future cloud formation and radiation feedback, we must know the mechanisms of particle formation. Therefore, we conducted a field campaign from March to August 2017 in Ny Ålesund, Svalbard at 79° N. Mass spectrometers were among the key instrumentation for solving the molecular mechanism of particle formation. In our campaign, we were able to solve the role of sulfuric acid, ammonia, amines, iodic acid, methane sulfonic acid, highly oxidized organic molecules as well as ions in new particle formation. To understand the effect of changing temperature on particle formation requires accounting for all different spheres. Based on our results, for example, we expect that changes in phytoplankton phenology and sea ice extent will greatly affect aerosol formation in those regions. This study aims to combine all the components related to gas-to-particle conversion necessary for predicting future behaviour of arctic clouds and climate.

7AP.30

Contrasting Physical Properties of Black Carbon in Urban Beijing between Winter and Summer. DANTONG LIU, Rutambhara Joshi, Chenjie Yu, James Allan, Hugh Coe, Michael Flynn, Junfeng Wang, Xinlei Ge, Yele Sun, Pingqing Fu, *University of Manchester*

Black carbon (BC) exerts both climatic and health impacts, especially in regional hot spots with high emissions. The populated megacity represents the most complex anthropogenic BC emissions where the sources and related impacts are very uncertain. This study provides a characterization of BC in the Beijing urban environment using single particle soot photometry during the joint UK-China APHH (Air Pollution and Human Health) project, in both winter (Nov. - Dec. 2016) and summer (May - Jun. 2017). During this experiment, we successfully gathered 4 weeks of continuous measurements for each season, including several severe pollution events in Beijing. The BC was found to have contrasting physical properties between both seasons. In winter, during periods of high pollution levels, the core sizes of BC were larger and the coatings were thicker; whereas in summer at the same level of pollution, core size of BC particles showed little variation and the coatings were lower than in winter. This phenomenon may result from a more significant contribution of BC from the residential emission sector in winter, but may be also modulated by local and synoptic meteorology. By measuring the BC physical properties in single particles, we separate four modes of BC with different size-resolved mixing state. By comparing these modes of BC with source apportionment results based on chemical composition analysis using soot particle mass spectrometry, we are able to link the separated BC modes with possible emission sources. This paper will examine the behaviour and contribution of BC with contrasting physical properties in both seasons and will link this to the optical properties to evaluate the possible mass contribution and optical budgets of BC among different emission sectors in Beijing.

7AP.31

Theory for the Glory. Extensions of the Surface Wave Mechanism. CHEYNE WEIS, Christopher Sorensen, *Kansas State University*

The optical phenomena of the glory has been explained in terms of the interference of beams emanating from surface waves from diametrically opposite sides of a spherical particle. This explanation clearly predicts a linear correlation between phase angle of the first maximum in intensity nearest to the back direction and the size parameter. We find a limitation to the refractive indices where this surface wave mechanism is viable, and then demonstrate through the Mie Solution that the correlation continues outside this domain, and then gradually deviates as the refractive index increases. For these larger refractive indices we then give an alternative mechanism based on ray optics (with no surface waves) possible at refractive indices above the square root of two that predicts the same functionality. Our non-surface wave glory, while of interest in itself, might have use for explaining the enhanced scattering that occurs for many non-spherical particles that occur in nature.

7AP.32

Molecular Content of the Critical Clusters of Lower n-Alkanes: Experimental Characterization Using Mass Spectrometric Detection and Small Angle X-ray Scattering. KEHINDE OGUNRONBI, Martina Lippe, Ruth Signorell, Barbara Wyslouzil, *The Ohio State University*

Understanding the vapor to liquid phase transition of n-alkanes is motivated by both technological and fundamental considerations. On the one hand, separation processes that recover natural gas liquid (NGL) from raw natural gas streams often involve expanding and cooling the natural gas stream across Joule-Thompson throttling valves, turbo-expanders, or supersonic nozzles. In all cases, vapor phase nucleation initiates condensation of the longer chain length alkanes. On the other hand, the simplicity of the interactions between n-alkane molecules makes them interesting candidates for both fundamental experimental and simulation studies.

In this work, we investigate the vapor-liquid nucleation of lower n-alkanes – pentane, hexane, and heptane – on the microsecond timescale in supersonic Laval nozzles and report the critical cluster sizes of droplets formed in the nozzles. We characterize the expanding gas mixture flow inside the nozzle using pressure trace measurements (PTM) and characterize the aerosols generated in the nozzle using small angle x-ray scattering (SAXS). Analyzing the SAXS and PTM data from different nozzles, characterized by different expansion rates, yields the supersaturation dependence of the nucleation rate, from which we determine the critical cluster sizes using the first nucleation theorem. The results from this conventional approach are compared with the results of directly characterizing the clusters in a uniform post-supersonic nozzle flow using mass spectrometric detection and soft single-photon by vacuum ultraviolet (VUV) light.

7AP.33

Errors in Nanoparticle Growth Rates Inferred from Measurements in Chemically Reacting Aerosol Systems. CHENXI LI, Peter H. McMurry, *University of Minnesota*

In systems where aerosols are being formed by chemical transformations, individual particles grow due to the addition of molecular species. Other processes, such as coagulation, may also lead to particle growth, but coagulation is a well understood process that is described by the coagulation integrals in the aerosol general dynamics equation. Growth, in contrast, is not always sufficiently well understood to be accurately described in models, especially for chemically complex systems such as the atmosphere. Processes including condensation & evaporation, acid-base reactions, organic salt formation, liquid phase reactions, and the accretion of two or more organic molecules to form a larger compound having lower volatility may contribute to growth. Efforts to improve our understanding of growth due to chemical transformations often focus on attempts to reconcile observed growth rates with values calculated from models.

However, because it is typically not possible to measure the growth rates of individual particles in chemically reacting systems, they must be inferred from measurements of aerosol properties such as size distributions, particle number concentrations, etc. For example, atmospheric nucleation leads to the formation and growth of a nucleation mode. Growth rates are sometimes assumed equal to the growth rate of the geometric mean size of this mode. However, this modal growth rate is also affected by self-coagulation of particles within the mode as well as condensation of smaller molecular clusters that are often not measured. To determine growth rates from such observations, it would be necessary to correct for the effects of coagulation on modal size. This complicates data analysis procedures and may require information that was not measured or is otherwise unknown for the system under study.

This presentation quantifies errors in growth rates obtained using methods that are commonly employed for analyzing atmospheric data. We analyze "data" obtained by simulating the formation of aerosols in a system where a single chemical species is formed at a constant rate, R. The advantage of this approach is that we understand the system perfectly, so can unambiguously determine true particle growth rates, which are due solely to condensation and evaporation. We examine the effects of a pre-existing aerosol and of evaporation. We show that the maximum possible error in measured growth rates occurs for collision-controlled nucleation in a single-component system in the absence of a pre-existing aerosol, wall losses, evaporation or dilution, as this leads to the highest concentrations of nucleated particles. Those high concentrations lead to high coagulation rates that cause the nucleation mode to grow faster than would be caused by vapor condensation alone. Scavenging by preexisting aerosol, wall losses, evaporation and dilution decrease concentrations of nucleated particles, thereby decreasing errors associated with coagulation. Although we do not explicitly study the effects of growth pathways other than condensation (i.e., contributions to growth by other chemical species or processes), they would lead to higher growth rates and therefore smaller relative errors in growth rates due to coagulation.

Our analysis is based on the non-dimensional formulation described by McMurry and Li (2017). This allows us to draw general conclusions that are independent of the chemical species and of the rate of aerosol formation. We show that for collision-controlled nucleation, the modal growth rate can be up to a factor of five higher than the true growth rate.

McMurry, P. H. and C. Li (2017). "The Dynamic Behavior of Nucleating Aerosols In Constant Reaction Rate Systems: Dimensional Analysis and Generic Numerical Solutions." Aerosol Sci. Technol. 51(9): 1057-1070. doi: 10.1080/02786826.2017.1331292.

7AP.34

Fractal Scaling of Soot Packing density Across Five Size Decades. PAI LIU, William Heinson, Rajan K. Chakrabarty, *Washington University in St. Louis*

Fractal aggregates in nature grow with a scaling dimensionality less than the spatial dimension. This results in their packing density (ϑ_f)–defined as the fraction of volume occupied by solid component–decreasing with increasing size R_g/a (aggregate radius of gyration normalized by average monomer radius). Fundamental questions remain regarding the scaling laws and physical mechanisms controlling the evolution of ϑ_f for the aggregates produced from combustion systems, especially after the onset of gelation. Here, we experimentally map the scaling of ϑ_f for soot aggregates across five orders of magnitude of R_g/a. The ϑ_f-R_g/a scaling relationship evolves through three successive regimes with distinct power-law exponents of -1.20±0.01, -0.58±0.06, and -1.31±0.14. The first cross-over agrees with the classical aerosol-to-gel transition theory. This agreement, however, breaks down at the second cross-over point, where a late-stage cluster-cluster aggregation of gel particles takes over.

7AP.36

Can Nanodroplets Shatter? YENSIL PARK, Kehinde Ogunronbi, Barbara Wyslouzil, *The Ohio State University*

Millimeter and micron size water droplets that freeze from the surface inward can build up enough internal pressure, due to the density mismatch, to explode. In our freezing experiment of n-alkane nanodroplets, we occasionally observe droplets that shrink far more than they should based on the expected liquid/solid density change. Furthermore, at the low temperatures involved, mass loss by evaporation should be negligible, even if the droplets reach their melt temperature.

Data from n-hexane nanodroplets is particularly intriguing. Here, nanodroplets formed in a supersonic Laval nozzle by condensation and then froze. The particles and the phase transitions were characterized using pressure trace measurements (PTM), Small Angle X-ray Scattering (SAXS) and Fourier Transform Infrared Spectroscopy (FTIR). In one case the carrier gas was pure Argon and in a second case the gas mixture contained 12 % CO_2. In both cases we observed a sudden decrease in droplet size and a corresponding heat release event. In the Argon case, the average droplet radius decreased by ~ 7.5 %, and in the presence of CO_2 the decrease was ~ 17.0 %. FTIR clearly confirms freezing in the pure Ar case, but not when CO_2 is present. Since n-alkanes are known to freeze from the surface inward if the chain length is long enough, it may be possible that gasses expelled from the crystal structure exert enough pressure to shatter these droplets despite their small size.

7AP.37

Hybrid Fractality and Formation Mechanism of Aerosol Gels. YULI W. HEINSON, William Heinson, Pai Liu, Rajan K. Chakrabarty, *Washington University in Saint Louis*

Aerosol gels are volume spanning, semi-rigid networks of solid nanoparticles possessing ultralow density and high surface area. The current consensus is that aerosol gels have a hybrid morphology with a mass (D) and surface (D_s) fractal dimension ~ 2.5 at super-micron length scale and ~ 1.8 at submicron length scale. In this study, we show that this consensus is partially complete and is not universal. Using our light scattering apparatus, we studied the structure factor of carbon aerosol gels produced using a buoyancy-opposed flame (BoF) aerosol reactor which facilitates continuous aerogelation on a millisecond time-frame. Our light scattering apparatus measured the scattered intensity by the gel particles in the scattering angle range of 1˚ ~ 168˚. We were able to probe the hybrid morphology by plotting the scattering intensity versus q, where $q=4\pi/\lambda \sin(\theta/2)$ with λ the wavelength and θ the scattering angle. Our light scattering results indicate that aerosol gel particles produced from our BoF reactor process a $D \approx 2.5$ and a $D_s \approx 2$. This surprising, yet previously undescribed morphology was further investigated for a convincing explanation using numerical simulation of diffusion limited cluster-cluster aggregates under varying monomer volume fraction conditions. This talk will present in detail our experimental findings and modeling interpretations.

7AP.38

Relationships between Scattering Directionality Parameters for Fractal Black Carbon Aerosols. APOORVA PANDEY, Rajan K. Chakrabarty, *Washington University in St Louis*

The magnitude of aerosol direct radiative forcing effect is significantly affected by the angular distribution of aerosol light scattering. In radiative transfer schemes, this distribution is typically condensed into single-valued parameters. An analytical expression known as the Henyey-Greenstein (HG) phase function is widely used to connect three single parameter representations of aerosol scattering directionality: the hemispherical upscatter fraction (β), the backscatter fraction (b), and the asymmetry parameter (g). The HG phase function does not take particle morphology into account, which could lead to significant errors for non-spherical particles. We calculated these single parameters for fractal black carbon (BC) aerosols using the numerically exact superposition T-matrix method. Here, we illustrate the effect of particle size and morphology on β, g and b for single particles. We developed empirical equations to capture the relationships between these parameters. For a known value of b, which can be obtained through direct measurement, the errors in β and g estimated using the HG phase function could be up to 35%. However, the large mass absorption cross-section of BC aerosols dominates their radiative forcing effect. Therefore, the rather large errors in scattering directionality result in ≤8% error in BC direct forcing efficiency at 550 nm wavelength.

7AP.39

Urban Aerosol Size and Concentration: Characterization in a Light Industrial Area 2017/2018 Compared to 2005.

TORSTEN TRITSCHER, Thomas Krinke, Axel Zerrath, Oliver F. Bischof, *TSI GmbH*

The particle size distribution of urban aerosols is typically dominated by ultrafine particles (UFP) originating from local sources such as traffic and industrial emissions. Due to their negligible mass they are clearly underrepresented by legislative PM10 mass measurements. This is one reason why the UFP contribution to urban air quality is better characterized by their number size distribution and particle number concentration.

In 2005 we carried out an initial study of the physical properties of the urban aerosol in a light industrial area in the city of Aachen, Germany (Bischof & Zerrath, AAAR 2005). The sampling location was near a freeway and in close proximity to two bus depots operating the local public transport network. We chose to repeat that study 12 years after the original campaign as the larger of the two bus companies frequently made upgrades to their bus fleet. This change in one of the predominant local emission sources should be notable in urban air quality improvements when comparing our latest measurements to the 2005 results. One interesting additional fact is that the city of Aachen introduced a low emission zone (LEZ) in February 2016. Other studies have shown (TROPOS, 2017) that improvements in air quality due to LEZ's are not well reflected when only considering PM10, while UFP measurements easily show reductions well in double digit values.

During both studies the sampling site was located at an identical distance of 50 m from the road and 200 m from the freeway. The depot of the public transport company and the lots of the private bus depot remained in their locations. Both result in extended bus traffic passing by the sampling location in particular in the mornings and afternoons of weekdays. We used a complete sampling system with PM10 head, PM1 cyclone, Nafion dryer and flow splitter in order to condition the ambient air aerosol and allow the connection of a wide choice of instruments.

An Ultrafine Particle Monitor (UFP, TSI Model 3031) was used to measure the particle number size distribution in 6 size fractions ranging from 20 to 800 nm. The UFP monitor was complimented by a high-resolution SMPS (TSI Model 3938) during selected periods. In addition we operated two models Condensation Particle Counters (CPC): a butanol-based monitoring CPC that fully complies with the CEN/TS 16976 specifications (TSI Model 3772-CEN) and a water-based instrument (WCPC, TSI Model 3788).

For the duration of the 2005 measurements the particle number concentration was typically below 5,000 particles/cm^3 at night time but exceeded values of 10,000 particles/cm^3 during day time with occasional peaks of up to 100,000 particles/cm^3. We found that these peaks correlated well with the bus fleet leaving from or arriving at the bus depot. Particle size distributions were dominated by particles below 200 nm in diameter and individual events with traffic revealed modal values of the distribution below 50 nm.

The influence of traffic remains clearly visible also in the 2017 data. Especially the morning peak when buses leave the depot showed a typical behavior, with the size distribution being dominated by particles smaller than 70 nm. The difference in total particle concentration between the UFP monitor and the CEN-CPC can be mainly attributed to the different lower cut-off size of 20 nm and 7 nm, respectively. We will present more detailed data, including measurements made during other months to complete the characterization of the urban aerosol at this site.

7AP.40

Glass Forming Properties of Secondary Organic Aerosol Tracers and Surrogates Examined by Thin Film Dielectric Relaxation Spectroscopy. YUE ZHANG, Shachi Katira, Jason Injae Jung, Peyton Spencer, Andrew Lee, Andrew Lambe, Wen Xu, Leonid Nichman, Manjula Canagaratna, Zhenfa Zhang, Avram Gold, John Jayne, Jason Surratt, Timothy Onasch, Douglas Worsnop, Paul Davidovits, David Chandler, Charles Kolb, *University of North Carolina at Chapel Hill*

Particulate matter (PM) has important effects on the climate, human health, and visibility. Field measurements from different parts of the world show organic components comprise more than half of the total PM mass loadings. Recent studies have shown that some organic particles can transform from a liquid/semi-solid phase state to a glassy phase state as temperature, humidity, and composition change. Glass transitions from liquid/semi-solid to solid phase states have important implications for reactivity, growth, and cloud formation (cloud condensation nuclei and ice nuclei) capabilities of secondary organic aerosols. Glassy particles are less likely to undergo heterogeneous reactions, thereby inhibiting particle growth due to the slow diffusion rates of surface reactants. Glassy particles are also more prone to form ice crystals, thus favoring cirrus clouds, compared with non-glassy particles.

The small size and relatively low mass concentration of SOA in the atmosphere make it difficult to monitor atmospheric SOA glass transitions using conventional methods. To circumvent these difficulties, we have adopted a new technique for measuring glass forming properties of atmospherically relevant organic aerosols. Aerosol particles to be studied are electrostatically deposited in the form of a thin film onto a quartz surface with interdigitated electrodes. The thin films were then analyzed by dielectric spectroscopy, which provides dipole relaxation information related to the motion of the molecules as a function of temperature (373 to 233K) at atmospherically relevant cooling rates. The glass transition temperatures (T_g) of organic aerosol components (glycerol and citric acid) are obtained using this technique, and the results agree well with available literature data.

The glass transition temperatures of isoprene SOA components, including isoprene-derived epoxydiols (IEPOX) and 2-methyltetrols, were measured at three atmospherically relevant cooling rates, 2 K/min, 5K/min, and 10 K/min. The glass transition temperatures of these two compounds range from 162-166 K and 240-245 K, respectively. The results indicate that increasing the cooling rate can reduce the glass transition temperatures of isoprene SOA tracers by 4-5 K. This temperature difference corresponds to an 800-meter height in the ambient atmosphere for the corresponding updraft induced cooling rates. These results underscore the importance of atmospheric variables (such as updraft rates) of organic particles on their phase state and subsequent multiphase reactivity and cloud formation properties.

The glass transition temperatures of water-organic binary mixtures were measured as five mixing ratios. The Gordon-Taylor equation is applied to fit the glass transition temperatures of the mixture, where 136 K is the T_g of pure water. The parameterization of the Gordon-Taylor equation is applied to calculate the effect of relative humidity (RH) and water content on the glass transition temperature of organic aerosols, assuming a growth factor of 1.2 at 90% RH. The glass transition temperature of organic aerosols drops by 15-20 K as the relative humidity changes from <5% to 90%.

In summary, the data obtained with broadband dielectric spectroscopy can be used to characterize glass transitions for both simulated and ambient organic aerosols. The glass transition temperatures of organic aerosols as a function of water content and cooling rates are derived, and their climate effects are interpreted.

7BA.1

Microbial Population Structure in Aerosols from Near-ground during Fog–haze Days in Northern China. YUNPING HAN, Mengzhu Zhang, Lin Li, Junxin Liu, *Chinese Academy of Sciences*

Fog–haze events exhibit an episodic tendency in China. Aerosol particles during fog–haze days can affect human health and cause several diseases, particularly respiratory diseases. As such, the properties of aerosols and their microbial composition have been extensively investigated. The microbial properties of aerosols from near-ground are of different states under various weather conditions. However, microbial populations in aerosols from human breathing height under special weather conditions, such as fog–haze days, have been rarely examined. In our study, microbial populations in aerosols from near-ground (1.5 and 20 m) were investigated. Aerosols were sampled during and after fog–haze days.

All aerosol samples were consecutively collected at 1.5 m (breathing height) and 20 m (height of no surrounding obstacles) above ground during and after fog-haze days in northern China (116.34° E, 40.0 1° N). An impingement airborne microorganism sampler (SKC BioSampler, SKC Inc. USA) was used to collect aerosols. Clone library was used to analyzed microbial population.

A total of 400 sequences for bacteria and 200 sequences for fungi were obtained. After alignment was completed, 7, 2, 22, and 15 OTUs were identified in HYP-FZB20, HYP-FZB1.5, HYP-CB20, and HYP-CB1.5 clone libraries, respectively, and 7, 13, 1, and 4 OTUs were determined in the 50 screened fungal clones from HYP-FZF20, HYP-FZF1.5, HYP-CF20, and HYP-CF1.5 clone libraries, respectively. Coverage analysis indicated that the aerosol libraries represented approximately 83.00%–99.00% of the total number of the examined clones. Thus, a dependable inventory of bacterial 16S rRNA and fungal 18S rRNA gene sequences present in aerosols is provided.

Results showed that the bacterial diversity in aerosols during fog–haze days was lower than that after fog–haze days. Proteobacteria alone and Proteobacteria with Firmicutes were respectively detected in aerosols at 1.5 and 20 m during fog–haze days. In addition to Proteobacteria and Firmicutes, Bacteroidetes alone and Acidobacteria with Verrucomicrobia were respectively found in aerosols at 20 and 1.5 m after fog–haze days. The fungal species observed during fog–haze days were completely different from those detected after fog–haze days. Ascomycota and Basidiomycota were respectively detected during and after fog–haze days. The distribution of microbial diversity in aerosols exhibited meteorological and site-associated variations. The same potential pathogenic microorganisms were detected at different heights during fog–haze days. This study on the characteristics of microbial population in aerosols could provide a comprehensive understanding of the factors causing the harmful effects of particles on humans during fog–haze days.

7BA.3

SenseNet Bioaerosol Collector Development. DAVID ALBURTY, Zachary Packingham, Andrew Page, Steven Graham, Ann Packingham, *InnovaPrep LLC*

DHS has begun development of an indoor systems approach to a high-performing but low-cost indoor environmental monitoring for bioaerosol threats. The intent is to overcome cost barriers to the deployment of a widespread commercial and government network of monitoring devices. These systems will provide early warning for critical infrastructure such as convention centers, office buildings, mass transit centers, sports venues and other areas. The system development approach considers the technical challenges of sensor placement through a modeling approach, and uses a triggered aerosol collector. The collector operates at 200 LPM and the sample is captured on a dry electret filter tape. A prototype system was developed and a demonstration test was conducted using Barcode Btk endospores. Following capture, the spores are eluted from the filter by a carbonated surfactant buffer solution termed Wet Foam Elution™. The expanded wet foam efficiently elutes particles from the filter and then quickly collapses into two mL of flat liquid. The collector system pulls a measured quantity of sample fluid from 35 µL to one mL from the sample and transfers it through a standard Luer lock interface to a PCR identifier that is networked to the overall system for an alarm decision and response. The design and development of the automated low cost per sample bioaerosol collector and the technical demonstration aerosol chamber testing will be presented.

7BA.4

Optical Trapping-Raman Spectroscopy (OT-RS) for Concurrent Characterization and Monitoring of Physical and Chemical Properties of Single Airborne Particles. ZHIYONG GONG, Yong-Le Pan, Gorden Videen, Chuji Wang, *Mississippi State University*

The study of physical and chemical properties of a microscopic object, such as a single particle, is made possible using optical trapping (OT) technology combined with other measuring techniques. Here we show a universal optical trap combined with Raman spectroscopy (RS) and microscopy imaging for single-particle studies. The universal optical trap is constructed using two counter-propagating hollow beams and is able to stably levitate single particles of a wide range of properties, such as transparent or absorbing materials, organic (polymers, bioaerosols, etc.) or inorganic constituents (carbon, silica, glass, etc.), and spherical or irregularly shaped morphologies. Both physical and chemical properties and their temporal evolution of the trapped particle can be characterized simultaneously using the integrated OT-RS and imaging system. We created three sample cases to demonstrate the analytical merits of the system: (I) a single particle with no change, (II) partially degraded over the measuring period, and (III) one part from the fragmentized single particle. The particles' chemical compositions, crystalline states, etc. are inferred from their Raman spectra, while their physical properties (sizes, shapes, morphologies, etc.) are revealed by images. This integrated OT-RS system provides a new approach to concurrently characterize and monitor physical and chemical properties of single micrometer-sized objects optically trapped in air.

7BA.6

Two-Step Laser Desorption/Ionization Mass Spectrometry of Individual Microorganisms by Single Particle Aerosol Mass Spectrometry (SPAMS). DAVID FERGENSON, Sean Kinahan, Joshua Santarpia, *Livermore Instruments Inc.*

A Single Particle Aerosol Mass Spectrometer (SPAMS) was used to generate real-time mass spectrometric data acquired from individual aerosolized non-pathogenic microorganism particles, analyzed by infrared desorption followed by ultraviolet ionization.

SPAMS is a technology whereby individual aerosol particles are analyzed in real-time, with a dual polarity mass spectrum acquired along with the aerodynamic diameter of each particle. This SPAMS is distinct from predecessor instruments in its simplicity, its ability to operate under high aerosol concentrations, and the number of aerosol particles that it can analyze per second. A SPAMS instrument is maintained under vacuum and aerosol particles are driven into its differentially pumped interface by atmospheric pressure. An aerodynamic focusing lens stack focuses the particles into a beam assuring that they arrive at the center of the source region of a dual polarity time-of-flight mass spectrometer. A single continuous-wave laser that is square in profile is oriented across the aerosol beam so that, when a particle crosses it, light scattered from that particle is detected by a photomultiplier tube. The duration of the light scattering indicates the velocity of the particle which is related to its aerodynamic diameter.

In a conventional SPAMS instrument, as the particle exits the laser, the cessation of detected scattered light is used to actuate a pulsed ultraviolet laser which is focused just below the scattering laser. The pulsed laser desorbs material from the particle and ionizes the material, with resulting ions analyzed by the mass spectrometers. Previous experiments involving the analysis of individual aerosolized microorganisms by SPAMS have demonstrated the technique's ability to discern genera and, in some cases, species across different growth conditions. However, the information available in the mass spectra was limited by the fragmentation of the molecules by the harshness of the desorption process. Several predecessor instruments to the SPAMS were modified with an alternate desorption/ionization process whereby the individual particles were first desorbed into the vapor phase by a CO_2 laser and then ionized using an ultraviolet laser in a second step, preserving molecular ion information intact. In this work, a SPAMS instrument was fitted with a 2-step desorption/ionization scheme and applied to the analysis of individual microorganisms.

7BA.7

Pathogenic Bioaerosol Detection in Under 30 Minutes. Robert Ferguson, Corinne Whitby, Dumbrell Alex, IAN COLBECK, *University of Essex, Colchester, CO4 3SQ, UK*

Deleterious health effects can arise following exposure to infective airborne microorganisms (bioaerosols). However, the risk of human exposure to bioaerosols remains difficult to quantify in real time. Currently, regulators rely on culture-based methods targeting only a single pathogen (i.e. *Aspergillus fumigatus*) as the industry's 'gold' standard. Such approaches are labour and time intensive, taking days to produce results. As the vast majority of microorganisms cannot be cultured these methods underestimate microbial loadings and key pathogens that may also be present are routinely overlooked. We present a tool for detection of specific bioaerosol pathogens in the field in less than 30 minutes.

Our method is based on isothermal amplification (LAMP) of DNA. LAMP is ideal for pathogen detection as it can identify one copy of a specific gene target in less than an hour [1]. The time from sample collection to result is under 30 minutes. We can achieve this as the result is shown by a colour change in the reaction mixture (no gel electrophoresis is required). Additionally the method is highly portable, no specialized equipment is required and a heat block can be used. LAMP is more sensitive than PCR; we have been able to identify < 5 *E. coli* cells without DNA extraction. The method is also highly specific due to the use of 2-3 primer pairs; we are able to target specific stains or pathogen virulence genes. The method can also be combined with fluorescent methods for real-time quantification in the field on battery powered platforms such as the OptiGene II and III. Currently, we are developing assays for the detection of key pathogens including *Aspergillus fumigatus* and *niger*, *E. Coli*, *Legionella pneumophila*, *Bacillus anthracis*, and *Bordetella pertussis*. The method can also easily be adapted to detect specific virulence genes (e.g. *E. Coli* STa) or antimicrobial resistance genes when taxonomic identification alone is not sufficient.

This method is one of a suite of tools we are developing based on high-throughput sequencing and chemical marker analysis which represent the next-generation of methods for in-situ biomonitoring of bioaerosols. We envisage that soon regulators will be able to detect and monitor key pathogens in real time.

[1] T. Notomi, H. Okayama, H. Masubuchi, T. Yonekawa, K. Watanabe, N. Amino, and T. Hase, "Loop-mediated isothermal amplification of DNA.," Nucleic Acids Res., vol. 28, no. 12, p. E63, Jun. 2000.

7BA.8

Liquid Air Sampler Bias on Bacterial Biodiversity. JOANIE LEMIEUX, Marc Veillette, Nathalie Turgeon, Caroline Duchaine,
CRIUCPQ, Université Laval

Air samplers are essential in bioaerosols study in order to concentrate and analyze the microbial content of the air. In some environments and circumstances, the air can be highly charged with bioaerosols and can contain pathogenic microorganisms such as bacteria, molds and viruses. Bioaerosols can cause diverse illnesses to exposed individuals. Obviously, field sampling is mandatory for exposure assessment studies.

Preliminary data from our laboratory showed a drastic underestimation of biodiversity (microbiota) obtained with a liquid sampler compared to sampling with electrostatic filter (*Veillette & al., American Society for Microbiology General Meeting-Microbe 2017*). A considerable bias may be inherent to the use of different types of air samplers, even when used side-by-side in a single environment. There are two possible hypotheses to explain this divergence in biodiversity obtained: preferential re-aerosolization and preferential sampling.

This study aims at studying preferential re-aerosolization after capture, that is defined by the tendency of a given microorganism to be lost during liquid evaporation occurring while liquid sampling with SKC Biosampler© (SKC Inc.). To study this phenomenon, SKC Biosampler© collection liquid (20 mls) was spiked (n=15) with known concentration of two bacterial strains (*Pseudomonas aeruginosa* and *Staphylococcus aureus*), in known proportions. The fate of the spiked bacterial mix during sampler operation was then followed (before and after 15 minutes, 12.5 L/min sampling). The evaporated liquid (2 mls) content was also captured using a filter (SKC 37 mm closed face cassette, 0.4 µm polycarbonate filter), at the exhaust, between the pump and the sampler. DNA was extracted from SKC Biosampler© liquid samples (*before* and *after*) as well as from the cassette filter and specific qPCRs were performed. *Pseudomonas/Staphylococcus* ratios were then compared throughout the experiment.

When looking at the relative ratios (**RR**) of *Pseudo/Staph* in the *after* samples and in the *before* samples :

[1] $\mathbf{RR}_{\mathbf{P+S,\ a/b}} = (Pseudo_{\mathbf{After}} / Staph_{\mathbf{After}}) / (Pseudo_{\mathbf{Before}} / Staph_{\mathbf{Before}})$

we demonstrated that *Pseudomonas* proportion increases with the use of the sampler (is enriched in the remaining collection liquid) whilst *Staphylococcus* proportion decreases in the remaining liquid.
Consequently, the respective ratios (**R**) of *Staphylococcus* and *Pseudomonas* in the exhaust-connected filter and in the before samples:

[2] $\mathbf{R}_{\mathbf{S,\ f/b}} = Staph_{\mathbf{Filter}} / Staph_{Before}$

and

[3] $\mathbf{R}_{\mathbf{P,\ f/b}} = Pseudo_{\mathbf{Filter}} / Pseudo_{\mathbf{Before}}$

showed that *Staphylococcus* is 4.1 times more enriched in the exhaust-connected filter than in the before liquid (is lost in the remaining collection liquid) when compared to *Pseudomonas* ratio ($\mathbf{R}_{\mathbf{S,\ f/b}} = 0.0118$ and $\mathbf{R}_{\mathbf{P,\ f/b}} = 0.0029$).

Then, when comparing the relative ratios of P*seudo/Staph* in the *after* samples and in the *before* samples[1] ($\mathbf{RR}_{\mathbf{P+S,\ a/b}}$) to the relative ratios of *Pseudo/Staph* in the exhaust-connected filter and in the *before* samples :

[4] $\mathbf{RR}_{\mathbf{P+S\ f/b}} = (Pseudo_{\mathbf{Filter}} / Staph_{\mathbf{Filter}}) / (Pseudo_{\mathbf{Before}} / Staph_{\mathbf{Before}})$

we are able to affirm that *Pseudomonas* is concentrated in the liquid sampler through sampling while *Staphylococcus* as a tendency to be re-aerosolized from the sampler.

Other bacterial strains are being studied to better understand the factors influencing the preferential loss observed. This project showed a different pattern of loss and concentration of two bacterial species, starting to solve the puzzle on the bias involved in liquid air sampling.

7BA.10

Improvement of Cell Extraction from Filters after Bioaerosol Sampling. INKEN SCHULZE-HESSING, Dierk Pöther, Udo Jäckel, *Federal Institute for Occupational Safety and Health*

The impact of bioaerosols on ecosystem dynamics and human health is becoming increasingly evident. Therefore, the microorganism concentration and the community structures of bioaerosols in the environment as well as on work places were intensively studied using different sampling methods. However, studies determining the efficiencies of bioaerosol sampling methods are rare. Thus, the aim of this study was to investigate recovery efficiencies of microorganisms from different filter types commonly used in bioaerosol sampling.

Five different microorganisms were applied on polycarbonate (P) filters as well as on glass (G) and quartz (Q) fiber filters. Following application the bioaerosol sampling was simulated and cells were extracted from filters with a paddle blender. The recovery efficiency was determined a) via total cell counting with the fluorescent DNA stain 4',6-diamidino-2-phenylindole and b) fluorometric quantitation of extracted DNA. Scanning electron microscopy (SEM) was performed to investigate detachment of bacteria from the filter surface.

Significant species-specific differences in recovery efficiencies were revealed. DNA quantitation showed that recovery efficiencies ranged from < 1% to 45%. For *Pseudomonas nitroreducens* applied onto P-filters it was shown that the low recovery rates were mainly the result of insufficient extraction from the filter and attachment of cells to the extraction bags in the paddle blender. SEM pictures revealed bacteria penetrating deeply into the G/Q-fiber filters. However, incubation of exposed G-fiber filters with Proteinase K directly before DNA extraction increased the recovery rates of *P. nitroreducens* cells significantly from < 1% to 69%. Moreover, the incubation with Proteinase K allows the extraction of all tested cells from G-fiber filters without significant species-specific differences in recovery efficiencies.

In conclusion, our study shows the necessity to investigate bioaerosol sampling characteristics to achieve a reliable assessment of bioaerosol exposure. The application of sampling methods with unknown sampling efficiencies may lead to problems in community analyses by concealing the real composition. We were able to show an improved method for cell extraction from filters allowing increased and species-independent recovery.

7BA.11

Development and Optimization of the Electrostatic Precipitator with Superhydrophobic Surface (EPSS) Mark III for Collection of Bioaerosols. TAEWON HAN, Nirmala Thomas, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

In our earlier research, we developed a liquid-based electrostatic precipitator with the superhydrophobic surface (EPSS Mark I and II) for bioaerosol sampling where airborne particles are deposited onto a narrow electrode (3.2 mm) covered by a superhydrophobic substance. The deposited particles are removed and collected by a rolling water droplet (a few tens of microliters) which results in high concentration rates. The Mark I featured a separate charger (commercially available ionizer) and collector, while the Mark II was a single-stage electrostatic precipitator (charger and collector placed in the same chamber). The Mark I and II versions showed high collection efficiency (~70%) for sampling airborne biological particles; however, a commercial ionizer used to charge incoming bioaerosols in Mark I resulted in particles losses as high as 50%, and the ionizer (for the Mark I) and the laboratory made ionizer (for the Mark II) produced high levels of ozone.

Thus, the latest version of EPSS (Mark III) has been entirely redesigned into a two-stage electrostatic sampler (separate charger and collector) for better control of charging process to prevent particle loss in the charger and to minimize damage to collected microorganism due to ozone production during ion generation. Mark III consists of a static air blender, a charger, a transition section, and a collector; it has a shape of a cylinder (1 inch in diameter and ~3 inches in length) and is made of a static dissipative material (Delrin). Also, our earlier developed and low-ozone-producing charger (wire-to-wire design) is integrated with a newly designed collector. This charger features a tungsten wire (0.003 inches in diameter and 1 inch in length) installed in the middle of the charging chamber and connected to high voltage. A ring of stainless steel (SS) wire 0.015 inches in diameter is installed on the inside of the charging chamber at the middle of the tungsten wire and grounded. The collector consists of a grounded SS cylinder (1 inch in diameter) inside the collection chamber and an SS collection rod (6/32 inches in diameter and 2.5 inches in length), which is positioned in the middle of the chamber and connected to a collection voltage. After completing the sampling, the collection rod is removed from the collector and transferred into a glass tube, and then the captured particles are easily extracted using a small volume of water (300-600 microliters) and by ultrasonic agitation for 30 min.

At this stage of development, the Mark III was tested at different collection voltages (-7 to -9 kV), while the charging voltage was fixed at +5.25 kV when challenged with 1 µm in diameter polystyrene (PSL) particles and at flow rates of 10 L/min. The sampler's collection efficiency was determined by measuring the number of particles deposited on the collection rod and the reference filter using mass-balance analysis by a fluorometric method. The collection efficiency was about 55-70% at the flow rate of 10 L/min, and ozone production was below 10 ppb. Further, physical efficiencies were optimized as a function of the collection rod size at different PSL particle sizes (0.5, 1, and 3 µm) and flow rates (10 to 30 L/min). Viability and culturability of cells collected by Mark III were investigated by using ATP bioluminescence, a ratio of Live/Dead cells (flow cytometry), and Colony Forming Units, and compared against that of the reference filter when sampling for 10 min and 8 hours.

7BA.12

Development of Wet-cyclone System for Highly Enriched, Continuous and Automated Bioaerosol Sampling in Real Time. YUSUNG CHO, Seung Chan Hong, Ki Joon Heo, Jae Hee Jung, *Korea Institute of Science and Technology*

According to recent studies, most of the modern people have indoor activities of about 80-90% of the total activity time. As a result, there is a growing interest and demand for increasing social interest in indoor air quality and working environment conditions. Also, it has been reported that the inflow of fresh air from the outside is not performed smoothly due to the airtightness and improper air conditioning system operation, and physiological symptoms such as a headache, drowsiness, dizziness, and concentration decrease are reported. In particular, bioaerosols in fine dust are closely related to various airborne infections such as allergies and respiratory diseases, which can have adverse health effects on humans. Although sampling equipment has been developed for predicting and controlling the risk of fine dust and bioaerosols occurring in various environments, the equipment capable of real-time measurement and analysis has not yet been studied. In this study, we developed a wet-cyclone system capable of liquefying and collecting fine dust and bioaerosol in real time.

The wet-cyclone used in this study used design variables to have high efficiency and low separation particle size of conventional wet-cyclone. Also, the flow ratio (concentration ratio) between injected gas and liquid in the fabricated wet-cyclone was optimized (Orsini et al., 2008). Polystyrene latex spheres (PSL) were sprayed to test the particle collection performance of wet cyclone. Based on the obtained collection performance, the collection performance against bioaerosols was compared with the conventional BioSampler. In addition, for real-time particle collection performance test, the concentration of abruptly changing bioaerosols was compared with UV-APS (Ultraviolet Aerodynamic Particle Sizer), a real-time measurement instrument.

The operating conditions were determined according to the flow ratio between the gas and the liquid injected into the wet cyclone. From this, the particle collection efficiency according to each operating condition was measured. As a result, a collection performance of >99% particle collection efficiency and <1% particle loss was obtained based on 1 µm particles. Also, the wet-cyclone performed in this study showed higher biological collection efficiency than the conventional BioSampler in the evaluation of biological recovery efficiency (*S. epidermidis*). This is because as the gas and liquid are continuously injected into the wet-cyclone, a thin liquid film can be formed on the inner wall of the wet-cyclone, thereby relieving the physical impact when the particles are collected and stably collecting it. Furthermore, the real-time particle collection performance showed that it is possible to sample the concentration that changes every 1 minute after spraying the bacteria (*S. epidermidis*). This shows a similar pattern to UV-APS, which shows excellent performance in collecting and analyzing bioaerosols including fine dust particles in the air, which changes in real-time in various environments.

Our system could be useful for rapid and accurate airborne bioagent detection and monitoring system as an inexpensive, simple, portable, and continuous bioaerosol sampler.

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7BA.13

Droplet Microfluidics Based Detector for Bioaerosols. BRIAN DAMIT, *Johns Hopkins University Applied Physics Laboratory*

Robust monitoring technologies for airborne microbes are critical to mitigate the health effects posed by environmental and agricultural bioaerosols, and biowarfare attacks. Limitations of current detectors (e.g. slow response time and expensive consumption of reagents) have compelled the development of new technologies. In this work, a detector was developed which applies droplet microfluidics to bioaerosol detection. Droplet microfluidics, a subfield of microfluidics, is based on the creation of picoliter/nanoliter droplets containing compartmentalized reagents and supports enhanced assays and fluidic manipulations. The bioaerosol detector here functions by precisely focusing aerosols directly into these droplets, and thus harness the benefits offered by a droplet microfluidics platform.

A breadboard detector system was constructed which consisted of an aerodynamic focusing lens, aerosol-focusing nozzle, custom microfluidic droplet chip, and fluorescence microscope. Computational fluid dynamic simulations and Lagrangian particle tracking modeling identified the optimal settings for aerosol focusing into the droplets. Preliminary experiments, wherein test PSL aerosols were focused and deposited onto solid substrates, demonstrated sub 200-µm spot diameters for aerodynamic sizes of 2-5 µm. After obtaining fine aerosol focusing, collection of aerosols in the droplets was achieved by positioning the chip below the focusing nozzle, forming a pinned air-liquid interface at the chip surface, and then focusing test aerosols into that interface. Real-time inspection via microscopy confirmed aerosol capture at the interface. The measured recovery efficiency of aerosols from the droplets was aerosol-size dependent and ranged from about 27% to nearly 100%.

Finally, to prove bioaerosol collection and detection, a droplet propidium iodide (PI) assay was performed: the system distinguished between *E. coli* and non-biological aerosols within 20 s of PI incubation. Overall, this work established the technique of direct collection of aerosols into a convenient droplet microfluidic platform for the purpose of rapid bioaerosol detection.

7BA.14

Continuous Bioaerosol Sampling Using the Super-hydrophilic Silica Coated Wet-cyclone System. YUSUNG CHO, Ki Joon Heo, Byoung Uk Lee, Jae Hee Jung, *Korea Institute of Science and Technology*

Recently, increasing attention has been paid to the relationship between hazardous respirable bioaerosol and human health. Thus, there is growing need to develop the portable bioaerosol detector that can provide the real-time and continuous bioaerosol information. Recently, the bioaerosol analysis techniques based on micro-electromechanical systems (MEMS) have been studied for the miniaturization of the bioaerosol sensor with the accurate and rapid response of target aerosol.

The cyclone system has been used extensively to collect and concentrate airborne particles by the cyclonic action of the fluid in the cylinder. In the 1960's, the development of a wetted-wall cyclone (called wet-cyclone) having nearly continuous liquid flow was started as a means of sampling a large volume flow rate of air (about 1,000 L/min). In recent years, the wet-cyclone system has been developed for the real-time bioaerosol sampler. In this system, the target bioaerosol can be concentrated in a small amount of sampling water. However, the non-uniform and unstable water film condition in the wet-cyclone can yield the significant increase of the particle wall loss. This undesired situation is caused by the unstable momentum balance between air to the liquid stream, the rapid evaporation of the liquid, and the hydrophobic status of the wet-cyclone inner surfaces.

In this study, we applied the super-hydrophilic treatment to the inner wall of wet-cyclone by silica nanoparticle coating to make uniform and stable liquid film. The wettability of the coated surface was evaluated through the water contact angle measurement. Also, the durability test of coatings was conducted from the comparison of the contact angle before and after the sonication process. Finally, the performance of the super-hydrophilic coated wet-cyclone system was evaluated regarding particle collection efficiency and particle wall loss. The collection efficiency was defined as the aerosol to liquid transfer rate. In this test, we used the two types of test aerosol, standard polystyrene-latex particles (PSL) and *S. epidermidis*.

The hydrophilic performance of the polycarbonate surface is gradually increased with silica coating concentration. Additional annealing process of the sample in the dry oven can increase the binding property of the silica nanoparticle film and the substrate; thus its super-hydrophilic property can be maintained despite the 10-minute sonication environment. Finally, the aerosol to liquid transfer rate was increased ~45% to ~99.99% after the super-hydrophilic coating treatment on the inner wall of wet-cyclone.

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7BA.15

Carbon Stable Isotope Probing Demonstrates Growth of Airborne Methanotrophs. VALDIS KRUMINS, Kevin Dillon, Donna Fennell, *Rutgers, The State University of New Jersey*

Outdoor air holds $10^4 – 10^5$ cells m^{-3}, which until recently have been assumed to be inactive while aloft. We have previously shown that airborne bacteria – outside of water droplets or other aggregates – express proteins and produce ribosomes in response to volatile organic substrates. Here we examine the activity of airborne methanotrophic bacteria using DNA stable isotope probing, and demonstrate that bacteria also are capable of growth (production of DNA) in bulk air.

Methanotrophic cultures were established from rinsate of a maple leaf (dominated by type II methanotrophs) and from an outdoor air sample (containing mostly type I methanotrophs). The cultures were enriched and maintained in minimal media using methane as the sole carbon source. For each reactor run, up to 2 L of liquid culture (fed ^{12}C methane) were concentrated by centrifugation and aerosolized into rotating aerosol bioreactors using a single pass aerosol generator (SPAG, CH Technologies, Westwood, NJ, USA). The 0.32 m^3 paired reactors hold cells aloft for days, and are equipped with on-board sensors for temperature, pressure, relative humidity, CO_2 and methane. After filling with bioaerosols, the reactors were amended with 1500 ppm_v methane. One of the paired reactors received ^{13}C-labeled methane; the other, unlabeled methane. The reactors were rotated at 3 rpm and held at at 22 ^oC for five days. At the end of incubation, ~10^7 cell-sized particles remained airborne. These airborne cells were collected onto 0.8 µm SUPOR membrane filters and immediately frozen (-80 ^oC). DNA extracted from the filters was ultracentrifuged (48,000 x g) for 48 hours on a CsCl gradient. The gradients were then separated into 24 fractions. The particulate methane monooxygenase gene (*pmoA*) and methanotroph-specific 16S rRNA genes (type I or type II methanotrophs, depending on the culture) were quantified in each fraction using real-time polymerase chain reaction (qPCR). In the reactors which received ^{13}C labeled methane, separate DNA peaks representing ^{13}C DNA and ^{12}C DNA were detected in the gradient; while in reactors receiving unlabeled methane, a single ^{12}C DNA peak was detected.

Detection of ^{13}C DNA in the reactors amended with $^{13}CH_4$ is evidence of production of new DNA and thus growth by airborne methanotrophs. The results suggest that microorganisms can metabolize methane, a potent greenhouse gas, while airborne.

7BA.16

Comparative Assessment of Conventional, Fluorometric and Molecular Biomarkers of Airborne Microbial Activity during Condensation Capture and Direct Filtration. MARINA NIETO-CABALLERO, Patricia Keady, Nicole Savage, Mark T. Hernandez, *University of Colorado Boulder*

While the field of aerobiology has experienced rapid growth over the last decade, technology is still lacking that enables engineers and scientists to accurately assess the identity, abundance and activity of airborne microorganisms—both indoors and out. Accurate bioaerosol assessment remains limited by conventional filtration and impaction methods that can compromise, or otherwise influence, the physiologic and metabolic state of airborne microbes, as they are collected from the atmospheric environment.

In response, emerging condensation capture technology was assessed for its ability to preserve bioaerosols in the same physiologic state they exist when suspended in the atmosphere. As judged by direct microscopy, culturing and genetic material content (DNA and RNA), the impacts of whole cell bioaerosol recovery using Condensation Growth Tube Capture ((CGTC), Aerosol Devices, Fort Collins, CO) was juxtaposed to conventional particle filtration. Under this scenario, a full-scale environmental chamber (ca. 11 m^3) was charged with well-characterized pure cultures of bacteria and fungal spores that have often been used to model the behavior of bioaerosols that are relevant to the built environment and environmental health (*Bacillus sp., Mycobacteria sp., Legionella sp.,* and *Aspergillus sp.*). With exception to spores that were dry-aerosolized from a desiccated state, vegetative cells, harvested from liquid culture, were introduced to the chamber air and allowed to age under controlled temperature and humidity conditions. Over several hours, airborne microbes were periodically and concomitantly collected using CGTC and filtration, while being counted, sized and characterized by cytometry using a conventional laser coupled with Ultraviolet Induced Fluorescence ((UVIF), InstaScope, DetectionTek, Boulder, CO).

Bacteria, while in their late exponential growth phase, were aerosolized for ten minutes using a 6-jet Collison nebulizer, reaching an initial concentration at or above 10^5 cells/L in the chamber air. These airborne bacteria were collected by CGTC directly in the following liquids that were continuously chilled to 4^oC: phosphate buffered saline and a genetic preservative (DNA/RNA Shield, ZymoBIOMICS, Irvine, CA). Cellular preparation (washing) and extended nebulization time had no effect on culturability, cell size or cell count.

A time-series of recovery experiments was performed at different humidity levels (30% and 80%). Samples were aseptically taken from CGTC wells for 10 minutes after 30, 60, 90, 120, 150 and 180 minutes of aerosol aging in the chamber, following the initial aerosolization. This provided a means to independently isolate and compare cellular deposition rates as judged by the different recovery methods. Direct microscopic and cytometric counts were in agreement with the time-series recovery of airborne DNA gene copy numbers, obtained using quantitative PCR (qPCR) with universal bacterial primers. Quantitative PCR steadily recovered between 3 and 4 fold higher gene copy numbers than its direct microscopic counterpart, consistent with whole cell microorganisms containing multiple copies of the target 16s rDNA gene. As anticipated, a significantly lower and age-dependent response was observed from the standard culturing of colony forming units (CFUs) on rich, broad spectrum agar (R2A). About 0.1% of the microorganisms aerosolized could be recovered as CFUs; however, culturable cells rapidly declined below detection (<60 min) while the optical methods indicated orders of magnitude higher airborne cell numbers, consistent with amplicons of (phylo)genetic DNA and RNA targets. The direct recovery of whole cells into genomic preservative, suggests the persistence of different RNA pools that can be used as a robust activity indicator in this time window. Moreover, the optical diameter of the airborne bacteria collected significantly diminished during aerosol aging as judged by aerosol cytometry and direct microscopy.

7BA.17

Development of an Immunoassay for Detection of the Nitrated Form of Allergenic Ragweed Protein (nAmb a 1).

COURTNEY SEFFENSE, J. Alex Huffman, *University of Denver, CO*

The frequency of allergic conditions has risen over the past several decades, particularly in urban areas. It has been hypothesized that one cause for this rise may be links between allergenic pollen and urban pollutants. For example, secondary pollutant gases ozone and nitrogen oxides have been shown to react with tyrosine residues within certain proteins and that these chemically modified proteins can increase their allergenicity.

Thus far, relatively little investigation has been directed toward the measurement of nitrated proteins in ambient aerosol, and so the hypothesis about the urban pollen allergy phenomenon has not been well tested. One reason for the lack of measurements is the high relative cost and complexity of techniques to detect and quantify nitrated allergens in atmospheric samples. Several papers approximately 15 years ago pioneered the investigation of nitrated proteins in ambient samples [1,2], but since that point little study has been focused on ambient field samples. Laboratory work over the last decade has focused on aspects of the chemistry of protein nitration and oligomerization, using the birch pollen protein Bet v 1 as a model [i.e. 3-5] and other related work has utilized the human protein lactoferrin as a model [6].

Franze et al. [1,2] utilized an enzyme-linked immunosorbent assay (ELISA) technique to detect and quantify nitrated protein material in ambient aerosol samples. Following this initial work, we have begun to develop a sandwich ELISA protocol for the selected detection of nitrated Amb a 1 (nAmb), which is a key allergenic protein in Ragweed pollen, a ubiquitous allergen in many areas of the United States and Europe. The assay entails sandwiching the protein to be detected (antigen) between two antibodies and detecting the change in color, which varies a function of the antigen concentration. Our initial work has focused on nitrated bovine serum albumin (nBSA) protein as an inexpensive antigen model as we optimize procedures. We have recently begun optimizing a parallel procedure to detect nitrated nAmb, toward the eventual goal of applying the assay to samples of airborne pollen collected in the field. We will discuss details of the ELISA protocols, discussing factors affecting reliability of assay calibration curves. Initial work testing both the nBSA and nAmb protocols shows encouraging results.

The work is being conducted as a part of an undergraduate research thesis by Courtney Seffense and is supported, in part, by the University of Denver Undergraduate Research Center (URC).

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7BA.19

Effects of Temperature and Water Condensation on the Sampling of Infectious Influenza H1N1 Virus Aerosol through Water-based Condensational Growth. MAOHUA PAN, Leah Carol, Aneal Mamane, John Lednicky, Arantzazu Eiguren Fernandez, Susanne Hering, Hugh Fan, Chang Yu Wu, *University of Florida*

Inhalation exposure to airborne influenza viruses can pose major health risks to humans and animals, and potentially result in significant economic losses. A 2017 study reported that up to 646,000 people in the word die every year of influenza. However, studies about sampling of airborne infectious influenza viruses are limited due to inefficiency of existing virus aerosol samplers, and the sampling conditions vary a lot considerably, making sampling results difficult to compare to each other. In prior studies, we demonstrated high collection efficiency for airborne infectious influenza H1N1 viruses by the VIable Virus Aerosol Sampler (VIVAS). The objective of this study was to evaluate the effects of temperature and amount of water condensed onto the collection liquid of SESI (Super-Efficient Sampler for Infectious virus, an improved version of the VIVAS) on the viability of the collected infectious influenza H1N1 viruses.

In controlled laboratory experiments, H1N1 influenza virus (80-120 nm) was aerosolized using a Bioaerosol Nebulizing Generator (BANG) and the aerosolized virus was collected by the SESI. This SESI is composed of four components: Conditioner, Initiator, Moderator, and Collector. Sampling temperatures (10, 20, and 33ºC) were pre-set for the Collector, whereas the moderator's temperature was adjusted accordingly to keep the accumulated collection liquid to minimum (< 0.1ml). During tests of the effects of volume of accumulated condensed water on virus viability, the temperature of the collector was kept at 10 ºC whereas the Moderator's temperature was changed from 6 to 14 ºC, which resulted in different amounts of accumulated water in the collection media. PBS with 0.5% w/v BSA Fraction V was used as the collection liquid, and Madin Darby canine kidney (MDCK) cells using a standard median tissue culture infectious dose (TCID50) assay was used to determine the infectious virus titer (#/mL) of Influenza H1N1 virus.

When the sampling period was 20 min, survivability of the influenza virus was higher when the collector temperature was 10 ˚C or 33 ˚C than at 20 ˚C. Further analysis is needed to explain this reproducible finding. The amount of water condensed onto the collection liquid during the 20 min sampling did not have significant effects on the viability of the infectious viruses, which suggest that this parameter need not to be taken into consideration for sampling infectious influenza viruses within 20 min. This is the first time the effects of sampling temperature and the amount of water condensed onto the collection liquid on the viability of infectious viruses are evaluated using a SESI.

7BA.20

Efficiency of a Biotrickling Filter to Reduce Bioaerosol Emissions from Pig Buildings. JONATHAN M. VYSKOCIL, Valérie Létourneau, Matthieu Girard, Ariane Lévesque, Caroline Duchaine, *Université Laval*

Pig pathogens are released into the air by the exhaust fans of livestock buildings and may consequently contaminate nearby barns. The development of strategies to reduce bioaerosol emissions is then required as preventive measures. Outgoing air filtration systems can be used to reduce the risk of spreading infectious diseases to other farms during viral or bacterial outbreaks. The present study aims to characterize the effectiveness of a biotrickling filter, an air treatment unit (ATU), developed by the Research and Development Institute for the Agri-Environment (IRDA) to reduce the bacteria and viruses emitted from a pig building. The biotrickling filter consists of an inert filter media which supports a microbial community continuously fed through a nutrient solution sprayed over incoming air. Bioaerosols were sampled isokinetically and simultaneously upstream and downstream of two biotrickling filters (field replicates) using two high volume air samplers (Coriolisμ Biological Air Sampler, Bertin Corp.). Data recorded during each sampling include the temperature of air before and after the ATUs, the air flow rate within the ATUs, and the relative humidity of air entering the ATUs. The samples were collected in the summer, fall, and winter. A culture-based approach and molecular biology analyses were used to monitor microbial concentrations and populations captured and emitted by the biotrickling filter. Preliminary results show an increase in culturable bacteria downstream of the ATUs, but a decrease in total bacteria (qPCR). *Clostridium perfringens*, *Enterococcus*, and *Escherichia coli* were quantified by qPCR. While *C. perfringens* and *Enterococcus* concentrations were below the limit of quantification, *E. coli* were detected in samples. Any factor associations with *E. coli* concentrations before and after the ATUs are yet to be resolved. Illumina MiSeq Next Generation Sequencing Biodiversity Analyzes will be used to determine if the biofilter bacteria are being released and examine pig pathogens that are being removed by the biotrickling filter. Quantification of archaea and porcine circovirus by qPCR will as well be conducted in the next months. Strategies to eliminate air contamination between pig buildings need to be developed and used in the field as air spreading of pig pathogens is possible and as biosecurity measures already in place are inefficient to eliminate the overall contamination risk.

7BA.22

A Further Investigation of Non-thermal Plasma Inactivation of Airborne Viruses Using a Newly Designed Coaxial Plasma Discharge. TIAN XIA, My Yang, Ian Marabella, Abby Kleinheksel, Eric Monsu Lee, Bernard Olson, Darrick Zarling, Montserrat Torremorell, Herek Clack, *University of Michigan*

Porcine Reproductive and Respiratory Syndrome (PRRS) is one of the greatest threats to modern pork industry. The virus has been detected in air more than 9 km downwind of infected swine. Applying HEPA filtration, the traditional bioaerosol control technology, to ventilation air supplied to hog barns involves structural retrofits to buildings that can be costly, in addition to the periodic replacement of used filters. Non-thermal plasmas (NTPs) are electrical discharges comprised of reactive radicals and excited species that inactivate viruses and bacteria with minimal pressure drop. Our previous experiments using a packed bed non-thermal plasma reactor demonstrated effective inactivation of bacteriophage MS2 as a function of applied voltage and power. The present study examined the effectiveness of the same reactor in inactivating aerosolized PRRSv and the effectiveness of a newly designed coaxial plasma discharge reactor in inactivating aerosolized MS2. A PRRSv solution containing ~105 TCID50/ml was aerosolized at a rate of 3 ml/min by an air-jet nebulizer and introduced into air flows of 5 or 12 cfm followed by NTP exposure in the reactor. Two impingers sampled the virus-loaded air flow at both upstream and downstream positions of the reactor. Subsequent TCID50 assay and quantitative polymerase chain reaction (qPCR) analyses of the collected samples determined the pre- and post-treatment abundance of infective PRRSv (in TCID50/ml) as compared with the abundance of the viral genome (qPCR), whether infective or rendered inactive by NTP exposure. An optical particle sizer measured upstream and downstream aerosol size distributions, giving estimates of aerosol filtration by the reactor. The results showed that PRRSv was inactivated to a similar degree as MS2 at the same conditions, with the 1.3-log inactivation of PRRSv achieved at 20 kV and 12 cfm air flow rate. Differential pressure across the reactor was minimal compared to HEPA filters and a consumer-grade ozone filter reduced residual ozone concentrations down to levels commensurate with the ambient laboratory environment. The results demonstrate the potential of properly optimized NTPs for preventing infiltration of PRRSv into hog barns with ventilation air. Having established MS2 as a conservative surrogate for PRRSv, the present study also examines the MS2 inactivation efficiency of a new annular non-thermal plasma reactor design equipped to vary the gap distance between the electrodes. The coaxial electrode configuration is expected to generate a more evenly distributed plasma discharge and be easier to model in future studies.

7BA.24

Investigation of Oxidation Effect in Inactivation by an Electrostatic Precipitator with Humidifier. TAKUMI YAZAWA, Munehiro Shiraisi, Akinori Zukeran, Risei Wada, Jun Sawai, *Kanagawa Institute of Technology*

An electrostatic precipitator (ESP) can eliminate and inactivate airborne microorganisms to improve indoor air quality. Therefore, the authors have investigated to inactivate microorganisms collected on a collection electrode in a two-stage type ESP. As a result, the inactivation effect was significantly improved by humidification 1).

In this study, experiments were carried out to investigate the process of improving the inactivation effect. The concentrations of ozone in the gas and the reactive oxygen speacies (ROS) reached the surface of collection electrodes were measured, and the oxidation effect of ROS on the collection electede was evaluated using a decolorization test paper dyed with indigo carmine.

The experimental ESP has a two-stage structure of a discharge section and an electrostatic section. The discharging section has a wire-and-plates configuration composed of a high-voltage application wire electrode and grounded plate electrodes. The electrostatic section has a parallel-plate electrode structure composed of a high-voltage application electrode and grounded plate electrodes. The discharging section was supplied with DC voltage of between -8.5 kV and -9.5 kV to generate corona discharge, whereby the discharge current was adjusted to 19 µA, which maintained the ozone concentration of approximately 1 ppm. The electrostatic section was supplied with DC voltage of - 5 kV to form an electrostatic field. The gas velocity was adjusted to 0.5 m/s, and the relative humidity (RH) was controlled between 5 % and 95 % using a hulnidifier. The ozone concentration was weasured using an ozone monitor at the downstream side of the ESP. In order to observe the distribution of ROS reached the surface of the grounded plate electrodes, the gel reagents reacted with ROS were located on the electrodes. The oxidation effect of ROS reached the electrode surface was estimated using decolorization test paper dyed with indigo carmine which was located on the plate electrode.

As a result, the ozone concentrations at the case with and without the humidifier were approximately 0.9 and 1.1 ppm, respectively. The concentration decreased by using the humidifier.

ROS distribution on the grounded plate electrode had a maximum value at the location under the wire electrode in the discharge section, and that decreased on the downstream side in the electrostatic section. The distribution in the case without humidifier was almost the same with that with humidifier. Thus,the ROS distribution were not influenced by RH.

However, the test paper dyed with indigo carmine in the case with the humidifier was decolorized on the downstream side from the wire electrode due to oxidation effect of ROS, althoug that in the case without the humidifier was not decolorized.

These results indicate that the improvement of inactivation effect with the humidifier would originate from that moisture or water droplets absorbing ROS such as ozone attached and be held on the electrode surface.

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7BA.25

Performance of Silver, Zinc and Iron Nanoparticles Doped Cotton Filters against Airborne E. coli to Minimize Bio-aerosol Exposure. Attarad Ali, Maohua Pan, TREVOR TILLY, Muhammad Zia, Chang Yu Wu, *Quaid-i-Azam University Pakistan, UF Gainesville USA*

Various designs of air-cleaning devices and filters are available to trap and deactivate aerosolized microorganisms that cause human diseases; however, there are limitations to these methods that still need to be resolved, including elevated pressure drop, decreased flow rate, short life-span, regenerative capacity, as well as fouling and clogging due to microbial proliferation. The objective of this study was to evaluate novel nanoparticle (AgCt, ZnCt, FeCt) doped cotton filters, developed in our previous studies, as biocidal filters for bioaerosol attenuation. To evaluate the biocidal activity of the nanoparticle impregnated filters, lab-generated E. coli aerosols were nebulized and were drawn through the filters and a BioSampler for comparison. The dryness of the aerosol affected the survival of bacteria collected on the filter. The relative humidity (RH) of the aerosol was varied from 20% to 90% using the control (cotton) filter, and the optimal RH for collecting maximum viable counts (colony forming units, CFUs) was found to be 50±5%. The permeability for untreated cotton filter was measured to be 3.38×10-11 m2 while that for the silver doped filter (AgCt) was slightly higher at 3.64×10-11 m2; meanwhile, the FeCt and ZnCt filters demonstrated comparatively lower permeability at 2.06×10-11 m2 and 1.86×10-11 m2, respectively. Overall, the permeability values of these filters were within the range commonly found for filter media used in industrial bag filters. The doped filters showed initial viable removal efficiency (VRE; 1 – downstream concentration/upstream concentration collected by the BioSampler) as 100% whereas the control filter was only 80.09±3.13%. Afterward, the nanocomposite doped filters retained their viable efficiency (~99%) for four filter cycles where they were used to collect E. coli, rinsed and oven dried, while the control filter demonstrated VRE of 76.6±3.2%. Among the three filters, the AgCt illustrated the maximum VRE (99.5±0.23). The relative survival fraction (RSF) was determined by comparing the viable counts of collected microbes from an untreated cotton filter and a doped filter. The maximum RSF of 0.033±0.006 was exhibited by FeCt followed by ZnCt and AgCt (0.015±0.005 and 0.0063±0.0005, respectively). The pressure drop of AgCt was also notably found low as compared to other two filters (ZnCt and FeCt) and even control as well. The physical removal efficiency (PRE) determined by an Optical Particle Counter was 99.9±0.7% for ZnCt, 97.4±1.2% for AgCt and 97.3±0.6% for FeCt, where the control (cotton) showed only 77.4±6.3% for particles >500 nm. Overall, these results suggest that nanocomposite doped filter media, particularly AgCt, can provide effective protection against airborne pathogens with a lower pressure drop, elevated collection efficiency, and better disinfection capability as compared to untreated cotton filters, which are all important features for practical biocidal applications. The metal ions released in extraction liquid (PBS) after each cycle of filter reuse were analyzed by inductively coupled plasma optical emission spectroscopy (ICP-OES) and will be reported in conference.

7BA.26

Development of a Novel Biomimetic Platform for Simulating Human Respiratory Infections. David Drewry, Brian Damit, FELIX SAGE, Julia Patrone, *Johns Hopkins University Applied Physics Laboratory*

Airborne respiratory infections (e.g. inhalation of viruses, bacteria, or fungi) pose a serious threat to global health and current methods for studying human physiological response fall short for agents untestable on humans. Current methods used to study airborne transmission consist of aerosol deposition directly onto in-vitro cell cultures or exposure to in-vivo and ex-vivo animal models. Although used extensively, animal models are expensive and experimental results are challenging to extrapolate a human response due to anatomical and physiological differences. In-vitro models lack a realistic delivery method for bioaerosols and the benefit of multicellular and whole organisms response. This research seeks to address these shortcomings through the development of an experimental platform that provides a more realistic insight into pathogenesis and delivery of aerosol particles to human cells. The platform consists of an additive manufactured, anatomically-realistic upper respiratory tract for an average human male. The airway includes the mouth, trachea, and bronchi (to the third bifurcation) coupled with “inserts” seeded with human A549 cells. Embedded at various locations in the cast, these inserts match the natural curvature of the respiratory tract and allow for bioaerosols drawn into the platform to deposit naturally on the cells. Initially, inserts without A549 cells were subjected to bioaerosol loading to examine aerosol deposition location and to establish dose during an aerosol challenge. Airflow through the cast was representative of inhalation during light exercise. Finally, inserts were seeded with viable A549 cells and exposed to a model bacterial agent (*Staphylococcus epidermidis*). Infectivity was evaluated through live-dead staining and fluorescent microscopy. This type of platform is an important innovation in modeling whole-organ systems that can be paired with recent advances in bio-printing on the path to creating organotypic test beds. This will allow researchers to perform experiments that are more cost-effective, and that more faithfully represent airborne infection in humans.

7CB.1

Chemical Characterization of Combustion Aerosols Related to Wood Combustion and Internal Combustion Engines.

THORSTEN STREIBEL, Hendryk Czech, Jürgen Orasche, Toni Miersch, Martin Sklorz, Johannes Passig, Olli Sippula, Jorma Jokiniemi, Benjamin Stengel, Bert Buchholz, Ralf Zimmermann, *University of Rostock and Helmholtz Zentrum Munich, Germany*

Combustion related aerosol emissions exhibit a considerable impact on human health and the climate. They contribute to a large extent to the formation of ambient aerosol, which is known to cause adverse health effects. Although the association between ambient aerosols and adverse health effects is very well established by epidemiology, it is still not well understood which aerosol fractions or properties are responsible for the observed effects.

For a better understanding of these interrelations, a thorough chemical characterization of the emitted aerosol from various combustion sources is of high importance. In the framework of the Virtual Helmholtz Institute HICE, several measurement campaigns have been carried out devoted to a comprehensive analysis of gas phase products and particles produced by different combustion sources. Utilized measurement techniques comprised on-line methods based on photo-ionization mass spectrometry for real time analysis of gas phase components, and filter sampling for particulate matter followed by chemical analysis using gas chromatography/mass spectrometry. A second analytical method for chemical characterization of particles consisted in a hyphenation between a thermal/optical carbon analyzer and a photo-ionization time-of-flight mass spectrometer.

For example, the consumption of fuel wood as a renewable energy source is rising in developing and industrialized countries because of environmental, economic and political aspects. Aerosol emissions of state-of-the-art wood combustion compliances, namely a logwood operated masonry heater with air-staged secondary air supply and a pellet boiler have been investigated. For the masonry heater, spruce and pine wood served as fuel. Pine wood emitted significantly higher amounts of organic compounds than spruce wood. The pellet boiler showed considerable lower emission factors with respect to organic substances. An interesting aspect was the observation from simultaneous exposure experiments with lung cell cultures, that compared to diesel exhaust wood combustion aerosol exhibited less severe biological responses on transcriptome and proteome level, although it emitted higher concentrations of aromatic species.

Aging of the emitted aerosol was realized by a flow-tube reactor to investigate the potential of wood combustion aerosol for the formation of Secondary Organic Aerosol.

A second combustion source consisted of a gasoline engine test bench. The engine was run with gasoline containing 10 % of ethanol and with E85, a mixture of 85 % ethanol and 15 % gasoline. Two driving cycles were applied, one reflecting urban traffic, the other driving with high velocities between 80 and 180 km/h for four hours. E85 showed much lower emission of particles and aromatic species, but high gas phase emissions of unconsummated ethanol and acetaldehyde. Driving with high velocities using E10 fuel led to a perceptible increase of polyaromatic hydrocarbons and carbon monoxide emissions.

7CB.3

Water Sorption Phenomenon on Aerosols Emitted during a Fire: Determination of the influencing Physico-Chemical Parameters.

LAURA LINTIS, Alexis Coppalle, François-Xavier Ouf, Cécile Vallières, *Université de Lorraine/IRSN*

Fire constitutes a hazard in a nuclear facility. It can lead to the clogging of HEPA (High Efficiency Particulate Air) filters by soots which are aggregates of carbonaceous primary nanoparticles. The presence of water leads to a higher filter airflow resistance. The water condensation on particles, initiated by an adsorption process, must be taken into account in order to better estimate the clogging process. This study consists in determining the most influencing physico-chemical parameters of soots on the adsorption phenomenon.

Combustion of isolated fuels heptane, PMMA and hydraulic oil has been carried out at analytical scale in a controlled atmosphere calorimeter cone. Fire tests were performed at two dioxygen concentrations: 21% and limit dioxygen concentrations before extinction in order to mimic the vitiated surrounding atmosphere occurring during a fire in a confined local. Online analysis including a SMPS (Scanning Mobility Particle Sizer) and ex situ physico-chemical analysis were carried out to determine the morphology, densities, specific surfaces and chemical surface compositions.

The CMD (Count Median Diameter) measured at 21% of dioxygen concentration presents values between 160 and 200 nm. A CMD diminution of 10% up to 50% depending on the fuel was observed for the minimal dioxygen concentrations. This aggregates CMD obviously influenced by dioxygen concentration is a parameter controlling the soot cake porosity during clogging processes. Transmission electronic microscopy pictures analysis lead to values of primary particles diameters of 30 and 36 nm for heptane and PMMA soots respectively. Unlike the aggregates CMD, these primary particle diameters do not change significantly with the dioxygen concentration. The elemental analysis leads to almost identical carbon amounts of about 90% at 21% of dioxygen concentration and show a diminution of 2% at the minimal dioxygen concentration. Organic carbon amounts are systematically higher for soots produced in a vitiated atmosphere. Heptane shows the most significant increase from 1% to 18%.

Water uptake has been measured at a constant temperature of 25°C for different relative humidity using a Dynamic Vapour Sorption Vacuum microbalance. As a preliminary step, water sorption measurements have been performed for two reference black carbons with primary particle diameters of 25 and 95 nm. Water uptakes of 10% for the lowest diameter and 1% for the highest highlighted a clear influence of this primary particle diameter on water adsorption. Identical water adsorption isotherms were obtained for samples compacted in pellet of 60% apparent porosity and left at looser powder state characterized by porosities close to 98%. It excluded the apparent porosity and indirectly the CMD as influencing parameters on sorption process. Soots present similar water uptakes of 3% at 90% of relative humidity. The isotherm shapes are characteristic of Vth type isotherm (*Rouquerol et al.*, 2014), reflecting a multilayer adsorption mechanism on hydrophobic adsorbents. However, water uptakes obtained at minimal dioxygen concentrations are systematically 0,5% higher than those obtained at ambient concentration. Those discrepancies can be explained by higher organic carbon amounts and lower carbon element amounts with the dioxygen concentration decrease previously indicated. The primary particle diameter was brought out as major influencing parameter on water sorption phenomenon occurring on soots.

For comparison, water isotherms of IIth type were obtained with realistic fire soots. They were collected on a HEPA filter during a large scale fire of a gloves box essentially composed of PMMA walls. The concave shape at low humidities is characteristic of high interactions with water. The water uptake increase up to 6% at a relative humidity of 90% reveals the beginning of the capillary condensation stage. Realistic soots have been found having a hydrophilic behavior compared to the soots produced at analytical scale.

7CB.4

Real World Emission Factors of Fine Aerosol and Carbonaceous Constituents from On-Road Transport in India. JAI PRAKASH, Dilip Ganguly, Gazala Habib, *Indian Institute of Technology Delhi*

Accurately measuring emission factors (EFs) are prerequisite for the correct emission estimates. The radiative forcing of carbonaceous constituents of aerosol (Elemental and Organic Carbon) are agreed to have significant climate implications over South Asia including India and China, where the abundance is high. However, a large discrepancy between model simulated and satellite retrieved absorbing aerosol optical depth was estimated in recent work by Bond et al (2013). The lack of knowledge on regional source activity, technological advances and unavailability of emission profiles of regionally important sources are stated as main reasons for such incongruity. For Indian on-road transport sector the emission estimates relied on EFs of PM2.5 measured either using chassis dynamometer following standard driving cycle or derived from emission models, and fraction of EC and OC adopted from literature for other countries. These EFs introduced an undefined uncertainty in recent emission inventories of road transport sector. None of the study has reported EC and OC emission factors for Indian vehicles. Therefore, for the first time, a technology based emission factors of OC and EC measured during on-road operation of vehicles in Delhi were used for refining the emissions estimates for the base year 2013. A logistic model was used with fixed parameters and vehicle registration data for the year 2013 to estimate the on-road vehicle population. The on-road vehicles were dominated by 2Ws, followed by 4Ws, others, LMVs-goods, HDVs-truck and buses with new vehicles comprising the majority of the on-road fleet. A portion of superemitter, which is highly unreliable, was assumed as 17% of the on-road population. Vehicle mileage and annual distance traveled were compiled from the literature and thus, fuel consumption was estimated at national level and disaggregated state to district level using vehicle population as proxy. Emissions of PM2.5, EC and OC were estimated as 260 (134-386) Gg y-1, 123 (65-181) Ggy-1 and 84 (37-130) Ggy-1 respectively. The PM2.5, EC, and OC emissions from the on-road transport sector for the base year 2013 contributed 7%, 17%, and 6% of total emissions from India. Another important finding of this work is new vehicles emit 70-80% of national level PM2.5 and EC compared to old vehicles, while old and new vehicle both equally contributed to OC emissions. The new emission factors from on-road measurement and emission estimates for on-road transport sector and its implications in climate forcing will be discussed.

7CB.5

Chemical Characterization of Biomass Burning Sources Using Targeted and Untargeted Approaches. CAMILLE NOBLET, François Lestremau, Jean-Luc Besombes, Olivier Favez, Serge Collet, Alexandre Albinet, *INERIS*

Biomass burning is a significant source of particulate matter (PM) in ambient air. To date, the evaluation of the distinct contributions of both, wood burning, used for residential heating, and green waste burning, on PM concentration levels is difficult and rarely achieved. Such discrimination is of major concern for air quality policy-makers in order to implement effective actions to reduce air pollution. The main objective of the research project SODEMASS (bioMASS burning SOurces DEconvolution) is to identify specific organic molecular markers and/or chemical patterns of both biomass burning sources that can be further used in PM source apportionment studies. Several experiments have been performed in “real” conditions using different wood combustion appliances such as a residential wood stove and a fireplace. Several parameters have been investigated including the output conditions (nominal vs reduced) and the wood log moisture content (mix of species including beech, oak, and hornbeam). In addition, green waste burning experiments have been carried out in a large combustion chamber facility (1000 m^3) using two kinds of burning material such as grass mowing with tree leaves and hedge trimming with branches. Several physicochemical parameters (smoke temperature, O_2, NO_x, CO, CO_2, non-volatile PM concentrations) were monitored continuously by using automatic sensors or analyzers and about 50 PM samples (on quartz fiber filters) have been collected after dilution of the channeled smoke (dilution factor about 1000). Filter samples have been characterized using both, targeted (levoglucosan and its isomers, methoxyphenols, alkanes, polyols, catechols and derivatives as well as EC/OC) and non-targeted (high resolution mass spectrometry (Q-TOF) coupled to GC or LC) approaches. The data treatment and statistical analysis will allow highlighting specific organic molecular species (exact mass, retention time, molecular formula, MS/MS fragmentation…) or chemical pattern candidates of each biomass burning source.

7CB.6

Waste Burning Tracers in Residential Wood Combustion Area in Estonia. HANNA LII KUPRI, Marek Maasikmets, Riin Rebane, Erik Teinemaa, Viktoria Voronova, *Estonian Environmental Research Centre*

Estonia's health impact assessment study has shown that due to the fine PM in an ambient air, people's life expectancy has shortened up to 13 months, with the highest decrease in city centers or areas with extensive domestic heating (Orru, 2011). During domestic heating, often incomplete combustion occurs causing the formation of polycyclic aromatic hydrocarbons (PAH).

One of the biggest fraction in Estonia's municipal solid waste (MSW) consists of different plastic materials. Major compound in the smoke from burning plastics include terephthalic acid (TA), used predominantly in beverage bottles and similar containers (polyethylene terephthalate - PETE), polystyrene (PS), polyporopylene (PP), etc. The specific key organic tracer for burning plastics found in atmospheric particle samples also include 1,3,5-triphenylbenzene, which occurs in regions where plastic waste is burned (Simoneit, 2005). This suggests that combustion of waste which is largely composite of plastic materials can be traced using the characteristic species detected in the smoke of plastics and refuse burnings (Kumar, 2015). Currently, there are only few available studies related to tracers for plastic waste burning in aerosols.

As Estonia has a well-organized MSW systems, it can be assumed, that people are not burning waste to dispose of it, but it could be considered more as an habitual behavior. According to the members of Estonia's Chamber of Chimney Sweepers, in addition to the wood, paper and cardboard waste, people also tend to burn Tetra Pak®'s, sanitary napkins, diapers, various plastic packages, shoes, textile etc. According to the Estonian Environmental Inspectorate, it is difficult to assess the exact number of people who still practice burning household waste since such activities are done clandestinely. Burning waste can also be an important contributor to particle pollution, because wood and wood chips account more than 90% of the fuel used for Estonia's residential heating. Therefore, it is an important topic to address.

Methods and results

The analysis of aerosol chemical composition (using Aerodyne Aerosol Chemical Speciation Monitor) were carried out during the winter period of 2016 and the full year of 2017 in Tartu's residential wood combustion (RWC) area and Lahemaa EMEP background monitoring station. PM10 and PM2.5 levels in ambient air were measured using beta ray attenuation (BAM 1020, MetOne) analyzers and for PM10 gravimetric measurements high-volume sampler (Digitel DHA-80) was used.

For analyzing terephthalic acid 24 h high-volume filters were extracted by sonication-assisted solvent extraction and then analyzed with liquid chromatography tandem mass spectrometry (LC-MS/MS). Chromatography was performed on a reversed phase column with methanol and 0.1% formic acid as chromatographic eluents. Gas chromatography mass spectrometry (GC-MS/MS) was used for analyzing heavy metals and PAH's. Heavy metals (Al, As, Sb, Cd, Co, Cr, Mn, Mo, Ni, Pb, Se, V, Fe, Zn, Cu) were analyzed on ICP-MS (Agilent series 7500).

Contrary to widespread bias, MSW combustion is not only a problem in developing countries, but it is also taking place in Europe. In this research, we have found that the packaging waste combustion in household heaters and stoves might be quite an important issue in some RWC areas. The analysis has shown a good correlation of TA, PAH and benzo(a)pyrene which may have been released to the environment during incomplete co-combustion of wood and waste materials. Analysis of filters from both stations also showed increased amount of TA and benzo(a)pyrene during the heating period and during summer when people make bonfires.

7CB.7

Toxicological and Chemical Characteristics of Fine Particles from Burning of Crop Residues in China. KIN-FAI HO, Jian Sun, Haiyan Ni, Jie Tian, Yongming Han, Junji Cao, Hsiao-Chi Chuang, *The Chinese University of Hong Kong*

Crop residue burning is a major source of fine particulate matter and arouses significant concern in China and worldwide due to its adverse impacts on environment and human health. Five types of crop residue (rice straw, wheat straw, corn straw, sugarcane straw and sorghum straw) were selected and burned in a laboratory combustion chamber to mimic the combustion process. Total 28 sets of $PM_{2.5}$ samples were collected to determine their chemical and toxicological characteristics. Human lung alveolar epithelial A549 cells were exposed to $PM_{2.5}$ at concentrations of 0, 20, and 150 µg/ml for 24 hours. The cell viability and toxicity were measured by the trypan blue dye exclusion assay and lactate dehydrogenase (LDH) / interleukin 6 (IL- 6) release, respectively. Burning of wheat straw emitted the highest level of $PM_{2.5}$ while sugarcane and sorghum straw emitted the lowest. Carbonaceous species, organic carbon (OC) and elemental carbon (EC), were the dominant components in all samples which contributed ~50% of $PM_{2.5}$ in total. The ratios of OC/EC from crop residue burning ranged from 8.8 to 31.0 which were significantly higher than those emitted from wood and fossil fuel burning. Potassium (K^+) and chloride (Cl^-) are dominant water-soluble ions from crop residues burning, with an average abundance of 6.4 ± 4.4% and 14.5 ± 8.2% in $PM_{2.5}$, respectively. Exposure to $PM_{2.5}$ at the concentration of 20 µg/ml to 150 µg/ml decreased cell viability and increased LDH / IL-6 release. Strong negative correlations were found between cell viability and OC ($R = -0.66$) and some heavy metals such as Cr, Mn, Fe, and Ba ($R < 0.65$). Moreover, OC, Cr, Mn, Fe and Ba also showed strong positive correlations with LDH and IL-6 responses. However, $PM_{2.5}$ samples emitted from burning of sorghum straw showed the lowest levels of LDH and IL-6 (150 µg/ml exposure) which may be due to the lower abundance of OC and heavy metals in $PM_{2.5}$. In conclusion, our data indicate that $PM_{2.5}$ emitted from biomass burning contained high concentrations of OC and toxic metals which were strongly correlated to cell viability and inflammatory responses. The findings suggest a need to control the burning of crop residues which can induce significant health impact on human being.

7CB.8

Particulate Emissions from Residential Biomass Hydronic Heaters. Patricia Fritz, Brian P. Frank, NICOLE VITILLO, Marilyn Wurth, Jake Lindberg, Shida Tang, Dave Guerrieri, Thomas Wainman, Gil H. LaDuke, Todd Crawford, Nathan Walz, *New York State Dept. of Health*

Currently, residential wood combustion units are certified for particulate emissions on the basis of mass emitted. Mass-based standards essentially ignore particle emissions in the ultrafine size range that contribute significantly to the number of particles emitted but make negligible contribution to particulate mass. To inform energy policy, and to identify potential mitigation strategies beyond reductions in PM mass, direct measurements of the particulate number concentration and size distribution of PM emitted from residential wood combustion units are needed.

We conducted a laboratory study of residential wood combustion devices in collaboration with an emissions testing group. Particle concentrations were measured over the size range of 10nm to 10um with a suite of instruments capable of providing fine time scale resolution (e.g., one second) to capture rapid changes in the exhaust particulates with changing operational loads. We selected instruments employing a variety of particle measurement technologies, including an aerodynamic particle instrument (Dekati, ELPI+), an electrodynamic particle sizer and counter (TSI Nanoscan SMPS), and an optical particle sizer and counter (TSI OPS3330) for characterizing particulate size distributions from appliances operated over changing operational loads. In addition to size resolved measurements, we also collected total particle counts using a condensation particle counter (TSI CPC3775), $PM_{2.5}$ particle mass using a portable nephelometer (Thermo pDR-1500), and estimated mass of selected carbon fractions (e.g., black, brown carbon) using a 7-wavelength Aethalometer (AE33) and a 3-wavelength Absorption Spectrophotometer (Brechtel TAP). We also obtained estimates of the lung deposited surface area of potentially respirable PM was also obtained (Partector, NSAM).

7CB.9

In-field Emission Measurements of Common Incomplete Combustion Sources in Africa. DAVID PFOTENHAUER, Evan Coffey, Didier Muvandimwe, Christine Wiedinmyer, Rex Alirigia, Ricardo Piedrahita, Desmond Agao, Ernest Kanyomse, Abraham Oduro, Michael Hannigan, *University of Colorado, Boulder*

Anthropogenic emissions of pollutants in Africa still remain highly uncertain, and the contribution of residential emissions, domestic sources, and incomplete combustion is large. As part of the Research of Emissions, Air Quality, Climate, And Cooking Technologies In Northern Ghana (REACCTING), in-field emission measurements of trace gases and particulate matter (PM) were taken from 41 common combustion practices in the developing world. These sources include commercial cooking, charcoal making, kerosene lighting, trash burning, and roadside traffic sites. Emission Factors for carbon monoxide, carbon dioxide, and carbonaceous particulate matter were calculated. The emission factors will be used to update emission inventories and fingerprint sources for future studies related to personal exposure and apportionment of ambient pollution.

7CB.11

Chemical Characterization of Particles Emitted from Engine Operated by Natural Gas and Propane. SANNA SAARIKOSKI, Jenni Alanen, Hannu Vesala, Rasmus Pettinen, Mia Isotalo, Sampsa Martikainen, Matthew Bloss, Minna Aurela, Teuvo Maunula, Kauko Kallinen, Jan Torrkulla, Hilkka Timonen, Topi Rönkkö, Kati Lehtoranta, *Finnish Meteorological Institute*

Natural gas (NG) is used globally as a fuel in engines because of its good availability, competitive cost and lower CO_2 emissions compared to conventional liquid fossil fuels. However, also NG engines produce gas and particle emissions that can have effect on environment and human health. In terms of particle emissions, particle mass emissions from NG engines are small compared to conventional diesel engines because of lower soot particle formation in combustion but particle number emissions from NG engines, especially nanoparticle emissions, are not necessarily small. Although NG is most widely used fuel gas, in some power generation applications it is more advantageous to use other gas compositions, like ethane and propane, instead of NG that is composed mostly of methane. Changing the gas composition is likely to alter the emissions from gas combustion and also its environmental and health impacts. The first objective of this study was to examine particulate emissions from the engine operated by NG and propane. The second aim was to investigate the influence of different catalyst systems (oxidation catalysts and Selective Catalytic Reduction, SCR) on exhaust particles emitted from the gas engine.

Gas engine measurements were conducted at the engine test facility of VTT Technical Research Centre of Finland. A spark ignited passenger car engine adapted for NG and propane was used. Two different catalyst setups were tested of which the first one consisted of a combination of an oxidation and a Selective Catalytic Reduction (SCR) catalyst, and the other setup included only one oxidation reactor. Exhaust gas temperature was varied from 350 to 500 °C and exhaust gas flow was 80 kg/h or 40 kg/h. The chemical composition of exhaust particles was investigated by using a Soot Particle Aerosol Mass Spectrometer (SP-AMS, Aerodyne Research Inc.). Additionally, particle number concentration and particle size distribution were measured by a variety of instruments. The potential of gas engine exhaust to form secondary particles was examined by Potential Aerosol Mass (PAM) chamber.

Primary particulate mass emissions from the engine operated by NG and propane were very small. Primary particles were dominated by organic matter that consisted mostly of hydrocarbon compounds. Compared to primary emissions, secondary particulate mass emissions from gas engine were larger. Chemical composition of secondary particles was similar to NG and propane being dominated by sulfate (~50 %) and organic matter (~40 %), and followed by ammonium (~4 %) and nitrate (~2 %). However, the concentration and chemistry of secondary particles were dependent on the engine and catalyst conditions.

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7CB.12

Properties of Carbon Particles Generated by Methane Decarbonization in Oxygen Deficient Gas Streams. Mohammad Javad Afroughi, Farjad Falahati, Larry W. Kostiuk, JASON S. OLFERT, *University of Alberta*

At a sufficiently high temperature, methane (CH_4) can be decomposed to solid carbon black ($C_{(s)}$), a feedstock for many industrial products, and hydrogen (H_2), which can be used as a carbon-free fuel. As such, methane decarbonization is viewed as a potential method to produce hydrogen (or heat or electricity if the hydrogen is used as a fuel) without CO_2 emissions. Furthermore, the solid carbon can be sold for use in industrial products; however, its value depends on the physical properties (i.e. size, morphology) of the carbon. Several methane decarbonization processes have been proposed including bubbling the methane through molten metal, heating the methane by a plasma, or in the hot products of combustion gases.

This study investigates the physical properties of carbon particles generated during decarbonization of methane in hot products of two different premixed flames. An inverted burner is designed to provide a rich, laminar, premixed flame of propane- and methane-air, with a total constant flow rate of 36.5 SLPM. The burner later injects methane co-flow to be decomposed within a closed quartz tube (20 cm in diameter and 68 cm in length). By placing ceramic blocks with axial concentric holes, a thermally insulated, reaction chamber of 4 cm diameter is created inside the tube. The formed products of decarbonization are discharged through an exhaust with two sampling branches. Measuring gaseous concentrations, a branch of products is dried and sent to a gas chromatographer (GC), while the other branch samples carbon particles with a nitrogen dilution system. Size distribution, effective density, and volatile mass fraction of particles are obtained with sequential arrangements of a differential mobility analyzer (DMA), catalytic denuder, centrifugal particle mass analyzer (CPMA), and condensation particle counter (CPC). Dilution ratios are calculated using simultaneously measured CO_2 concentrations in exhaust products and diluted samples. Axial temperature distribution in the reaction chamber is also measured by a K-type thermocouple.

Different flow rates of methane (0.5 to 5 SLPM) are injected in oxygen deficient gas stream of propane- and methane-air premixed flames, with maximum temperature of 1170 and 1135 °C, respectively, to be decarbonized. Results show that properties of generated particles are strongly dependent on type of the premixed fuel, and decarbonized methane flow rate. Generally, decarbonization using propane-air premixed flame produces larger particles with higher number concentrations, for a given injected methane flow rate; e.g. total particle number concentration and median mobility diameter increase from 1.27×10^8 to 1.69×10^8 cm^{-3} and from 21 to 58 nm, respectively, due to change of premixed fuel from methane to propane at a constant decarbonized methane flow rate of 0.5 SLPM. Furthermore, median diameter of size distribution is inversely proportional to decarbonized methane flow rate, and decreases from 58 to 18 nm (21 to 18 nm) following the injection of 0.5 to 5 SLPM of methane to the propane-air (methane-air) premixed flame. It is also notable that effective density and volatile mass fraction of particles are size-dependent and decrease from ~2000 to 500 kg m^{-3} and from ~0.55 to 0.35, respectively, with the increase in mobility diameter from 14 to 700 nm.

7CB.13

A nvPM Formation and Oxidation Semi-Empirical Model for Gas Turbines in Commercial Aviation. Joseph Abrahamson, RANDY VANDER WAL, *Penn State University*

Several semi-empirical relations have been developed to estimate nonvolatile particulate matter (nvPM) mass emissions from rich-quench-lean (RQL) style combustors employed predominantly in the current aviation fleet. The accuracy of such methodology has been hindered by inaccurate combustor conditions. Additionally, current relations are not optimized for direct cruise nvPM emission predictions and do not account for fuels, in particular alternative jet fuels with reduced aromatic contents. An improved semi-empirical kinetic based predictive relation has been developed for these purposes. Accurate engine conditions are based on proprietary engine cycle data for a common RQL style combustor. Nonvolatile particulate matter formation rates dependent on equivalence ratio, thrust, and fuel components are developed to accurately predict emissions across thrust settings and fuels. The new model captures both ground and cruise altitude emissions. To incorporate fuel effects hydrogen content is used as it encompasses all three fuel components: aromatics, paraffins and cycloparaffins. Predicted values are validated against field campaign data collected over a decade from NASA Langley’s Aerosol Research Group with inclusion of cruise data.

7CB.14

CAAFCER: Particle Number Emission Factors from In-Flight Aircraft Fueled with Jet A1 and Biofuel Mixtures. STEVEN TRAN, Jason S. Olfert, Anthony Brown, Fred J. Ghatala, *University of Alberta*

The aviation sector has begun using biofuels to reduce greenhouse gas (GHG) emissions in an effort to fight climate change. The use of biofuels also has impacts on aircraft particle emissions. The Civil Aviation Alternate Fuel Contrail and Emission Research (CAAFCER) project was designed to investigate the emission performance of high blend Hydrotreated Esthers and Fatty Acids (HEFA) biojet and conventional Jet A1 fuel in a real environment via flight emissions monitoring and fuel analysis from passenger airlines under contrail conditions. While the particle emissions of biofuels have been studied extensively in laboratory conditions (with emissions sampled from engines or stationary aircrafts on the ground), few studies have been undertaken with aircraft emissions sampled in the air during commercial (revenue) flights.

In CAAFCER, the source of emissions came from Air Canada A320 series aircrafts with NRC's CT-133 trailing behind to collect contrail data. The Air Canada flights were travelling between Toronto and Montreal. The Montreal-Toronto flights used the biofuel blend while the Toronto-Montreal flights used Jet A1 fuel. The CT-133 flew in and out of the contrails in order to capture contrail and background data. The NRC CT-133 was equipped with the necessary equipment to collect contrail and emissions measurements such as a TSI 3776 ultrafine particle counter (lower limit of 2.5 nm), TSI 7610 particle counter (lower limit of 10 nm), Thermo 42I NOx Analyzer, LII300 black carbon sensor, FSSP-100 ice particle sensor and LiCor 840A CO2 and water vapour sensor. A thermal denuder (Catalytic Instruments) with a bypass was installed upstream of the 3776 CPC. The thermal denuder allowed for the measurement of non-volatile particles and was only installed in-line to the 3776 CPC.

Particle number emission indices for particles greater than 2.5 nm (3776 CPC) and greater than 10 nm (7610 CPC) were calculated to evaluate the emission performance of Jet A1 and biofuel using the Fuel Flow Method 2 developed by Boeing. This method relates fuel flow to emission indices which are both publicly available. NOx emissions were used as a tracer to determine the dilution ratio of the contrail between the source aircraft and the CT-133 measurement aircraft. The dilution ratio was then applied to the concentration of particles measured by the particle counters to estimate the total number of particles emitted by the source aircraft.

Final results will include emission indices for both the 3776 CPC and 7610 CPC. The emission indices for total particles (volatile and non-volatile) greater than 10 nm will be calculated for the biofuel blend and Jet A1 fuel. The emission indices for particles greater than 2.5 nm will be calculated for both types of fuel as well as total and non-volatile samples for each type of fuel.

7CB.15

PM2.5 and Its Carbon Components Emitted from a Diesel Engine Generator Fueled with Waste Cooking Oil-based Biodiesel Blends. Jen-Hsiung Tsai, SHUI-JEN CHEN, Chia-Chin Wu, Kuo-Lin Huang, Jia-Twu Lee, Wen-Yinn Lin, Chih-Chung Lin, *National Pingtung University of Science and Technology*

Diesel particulate matter (DPM) is typically composed of carbon particles (soot) and numerous organic compounds produced by incomplete combustion. DPM will cause serious air pollution and human health problems and it is also one of the major sources of fine particles ($PM_{2.5}$) in many urban areas. Till now, the $PM_{2.5}$ from non-road diesel generators fueled by waste cooking oil-based (WCO) biodiesel blends has seldom been studied. In this study, a small diesel generator, fueled with three WCO-biodiesel blends (W0 (pure diesel), W20 (20% WCO-biodiesel + 80% diesel), and W40), was operated at 1.5 and 3.0 kW loads to investigate the $PM_{2.5}$ and its carbon components in the exhaust. The results showed that the $PM_{2.5}$ concentrations in engine exhaust ranged from 12.9–15.9, 11.3–13.2, and 12.5–14.7 mg/Nm^3, and averaged 14.2±1.44, 12.1±0.86, and 13.4±0.97 mg/Nm^3 using W0, W20, and W40, respectively, at 1.5 kW. At 3.0 kW, the high $PM_{2.5}$ levels were 23.2–27.2 (average: 25.2±1.69), 15.1–22.3 (average: 17.9±3.45), and 17.9–20.6 mg/Nm^3 (average: 19.2±1.23 mg/Nm^3) using W0, W20, and W40, respectively. The $PM_{2.5}$ emission reductions were 15.2% and 6.07% at 1.5 kW, and 31.8% and 23.8% at 3.0 kW, using W20 and W40, respectively. Under the two loads, the concentrations of $PM_{2.5}$-bound organic carbon (OC) and elemental carbon (EC) were 3.58±0.94 to 6.50±0.29 mg/Nm^3 and 9.12±0.38 to 16.2±0.87 mg/Nm^3, respectively, for using W0, which were lower than those for using W20 by 23.7–45.4% and 6.85–21.4%, respectively (OC = 2.73±0.66 to 3.55±0.69 mg/Nm^3 and EC = 8.50±0.14 to 12.8±2.87 mg/Nm^3), and those for using W40 by 17.0–38.5% and 4.69–38.5%, respectively (OC = 2.97±0.23 to 4.00±1.14 mg/Nm^3 and EC = 8.69±0.13 to 13.2±0.53 mg/Nm^3). On average, the total carbon (OC+EC) contributed ~88% (OC and EC: 22% and 66%, respectively) of the $PM_{2.5}$ mass concentration.

7CB.16

PM2.5-bound Metal Emission from a Diesel Engine Generator Fueled with Biodiesel Converted from Used Cooking Oil.

Jen-Hsiung Tsai, SHUI-JEN CHEN, Chi-Ying Hsieh, Cheng-Hung Tsai, Wen-Yinn Lin, Kuo-Lin Huang, Chih-Chung Lin,
National Pingtung University of Science and Technology

Many studies have confirmed that the use of appropriate proportion (~20 vol%) of the biodiesel converted from non-edible greases (e.g., waste cooking oil (WCO)) can effectively reduce the emissions of particulate matter (PM), traditional gaseous pollutants, polycyclic aromatic hydrocarbons (PAHs) and other pollutants of diesel engines. However, some poor-quality aluminum, copper or stainless cooking utensils may result in the presence of toxic metallic elements (e.g., Ni, and Cr) in recycled WCO. Therefore, the emission of particulate toxic metals from the combustion of WCO-based biodiesels needs to be investigated. This study presents the emissions of 21 metals (Na, Mg, Al, K, Ca, Ti, V, Cr, Mn, Fe, Ni, Cu, Zn, As, Sr, Mo, Cd, Sn, Sb, Ba, and Pb) in the emitted $PM_{2.5}$ from a small diesel generator, fueled with WCO-biodiesel blends under 1.5 and 3.0 kW loads, by adopting $PM_{2.5}$ cyclones to separate aerodynamic particle sizes ≤2.5 µm from the larger particles in the tailpipe stream. A brand of pure fossil diesel (W0) was adopted as the base fuel, and it was added by 20% and 40% WCO-based biodiesel to form W20 and W40 blends, respectively. The results showed that the mean concentrations of the sum of 21 metals (ΣMetals) on the $PM_{2.5}$ in the exhausts for using the tested fuels followed the order W40 (60.8–109 $\mu g/Nm^3$) < W20 (66.9–110 $\mu g/Nm^3$) < W0 (81.7–142 $\mu g/Nm^3$), despite the generator loadings. Additionally, the mean contents of ΣMetals were in the order D100 > W20 > W40 at 1.5 kW and W20 > D100 > W40 at 3.0 kW. Regardless of fuel blends, the mean concentrations and contents of ΣMetals on $PM_{2.5}$ increased as the engine loading increased. The metal elements in $PM_{2.5}$ sample were dominated (over 90% mass of total metals) by Na (3.20%), Mg (5.31%), Al (4.65%), K (19.0%), Ca (20.9%), Fe (10.5%), and Zn (31.5%). The major contents of the rest (minor) metals were Ni (2.14%), Ti (0.74%), Cr (0.57%), Mn (0.55%), and Mo (0.41%). The reduction rates of ΣMetals for using W40 were 25.6% and 23.0% at 1.5 and 3.0 kW, respectively, while for using W20 the corresponding data were 18.0% and 22.6%, respectively.

7CB.17

Origin of Soluble Iron from Low-emitting Automobile Exhaust. JOSEPH SALAZAR, Benton Cartledge, Lynn Russell, Allen Robinson, Greg Drozd, Allen H. Goldstein, Brian Majestic, *University of Denver*

Soluble iron has been found to be a limiting reagent for phytoplankton in most of the southern oceans. Phytoplankton is a vital part of the ocean's ecosystem as it is involved in CO_2 uptake and nitrogen fixing. Thus, understanding iron geochemical cycle is essential to understanding the earth's oceans and atmospheric interactions. Soluble iron has been correlated to oxalates, nitrates and sulfates resulting in the hypothesis that iron is solubilized through an acid processing mechanism. Despite the correlations in field studies, these relationships have not been reliably proven in the laboratory. Previous field studies have linked soluble iron over the ocean to combustion sources and, in general, relative soluble iron tends to be greater in urban areas. To understand the origin of soluble iron in urban areas, PM was collected from the tail pipes of low emitting gasoline vehicles at the CARB dynamometer facility using the California Unified (UC) Drive Cycle. The PM was collected from the exhaust pipe and analyzed for inorganic ions, EC/OC, total and soluble metals, functional groups, and GC-MS was used to quantify the class of 11 to 18 carbon intermediate volatility organic compound (IVOC), ultimately categorized as alkane (ALK), single ring aromatic (SRA) and general (GEN) for each number of carbon. The results showed that the tested automobile emissions have a high fraction of percent iron solubility ranging from 0% - 81.9% with an average of 26.7%. This is a significant increase compared to crustal sources where the soluble iron is approximately 1% of total iron. The samples were analyzed by x-ray near edge absorption structure (XANES) spectroscopy, which confirmed that only Fe(III) was present in the samples and, thus, any increased solubility was not due to the presence of the more soluble Fe(II). Correlation of soluble iron to sulfate was insignificant (R2 = 0.157), as was the correlation to every measured chemical component, except one class. Soluble iron was highly correlated to the C11 - C18 IVOCs, with R2 values as high as .981 for IVOC SRA-C14. These results imply that the large driver in soluble iron from gasoline vehicle emissions is related to the organic fraction of the PM, suggesting that further studies are required to study metal-organic interactions in PM.

7CB.18

On-Line Measurements of Selenium Emissions from an Operating Coal Fired Power Plant. Edward Fortner, Joseph Roscioli, Jordan Krechmer, Manjula Canagaratna, Scott Herndon, JOHN JAYNE, *Aerodyne Research, Inc.*

Coal fired power plants are a significant emission source of criteria gas pollutants as well as trace elements. Volatile toxic elements pose special concerns since they may not be efficiently removed by existing gas phase control measures in modern power plants and can therefore pass through the different process streams and be emitted into the environment. While some elements such as sulfur and mercury have regulatory emission controls imposed others do not. One such element is selenium which is believed to exist mostly in the oxidized form. Selenium dioxide has received special attention since it has volatility characteristics that allow it to partition between the gas and condensed phases at typical flue gas exhaust temperatures. The relatively high volatility has made it difficult to quantify the fate of selenium using standard analytical filter based collection methods. Prior measurements of selenium in the flue gas have shown wide variability in material balance closures indicating an incomplete understanding of the behavior of selenium in the process stream. Here we present results from a field measurement project that demonstrates the use of advanced technology instrumentation for the real-time, on-line detection of trace pollutants from an operating power plant. Both mass spectrometric and infra-red spectroscopic instrument systems were used to measure the concentrations of selenium dioxide in the flue gas and to estimate gas-particle partitioning, emission indices and removal efficiencies. To our knowledge this was the first time such measurements have been made at an operating power plant with these instrument technologies and demonstrates their applicability for use in collecting chemically speciated data from power plant streams in real-time.

7CB.19

Collection Characteristic of Diesel Nano-Particles in an Electrostatic Precipitator: Experiment Using Residual Fuel Oil and Light Fuel Oil. HIDETOSHI SAWANO, Akinori Zukeran, Yasumoto Koji, *Kanagawa Institute of Technology*

Diesel engines have been extensively used as a generator, an automobile or an agrimotor due to low CO_2 emission. However, their exhaust gases contain air pollutants, such as NO_x and particulate matter (PM). It is known that nano-particles are included in PM. SO_x is also included in exhaust gas, when residual fuel oil is used.

The purpose of this study is to remove PM using an electrostatic precipitator (ESP). In particular, the relationship between nano-particle collection efficiency and the particle diameter was investigated for emission gas from diesel engine with residual fuel oil and light fuel oil.

The experimental system consisted of a diesel engine (displacement 400cc) and an ESP, and residual fuel oil (ENEOS LSA heavy oil (01)) or light fuel oil (ENEOS gas oil) were used for the diesel engine. The ESP has a needle-to-cylinder electrode structure with a metal cylinder with an inner diameter of 58 mm and a stainless steel needle electrode with a diameter of 1.6 mm (tip angle 14 °, curvature radius 22 μm). The voltage applied to the needle electrode was DC-16 kV.

A portion of the gas was drawn at the gas temperature of 160℃ and 10-hold diluted by the diluter at the same temperature of the gas. After cooling to the room temperature, the particle concentration was measured using a scanning mobility particle sizer (SMPS, TSI, Model 3936). SMPS can measure the particle concentration for the particle diameter between 5.9 and 250 nm. The collection efficiency η was calculated by equation (1):
$(1-(N/N_0))\times 100\%$ (1)
where, N is particle density after applying the voltage, and N_0 is particle density before applying the voltage.

When residual fuel oil was used for a diesel engine, the particle size distribution at the voltage of 0 kV had a peak of approximately 6.0×10^6 parts/cm^{3}at the particle size of 57 nm. At the voltage of -16 kV, the particle concentration at 57 nm decreased to approximately 2.2×10^5 part / cm^3. The collection efficiency was greater than 95%. This is due to electrostatic precipitation effect. However, the concentration for the particle size less than approximately 20 nm increased at the voltage of -16 kV in comparison with that at 0 kV. Thus, the experiment using the light fuel oil was carried out in order to investigate this cause. As a result, the particle size distribution at the voltage of 0 kV had a peak of approximately 6.6×10^6 parts / cm^3 at the particle diameter of 71 nm. At a voltage of -16 kV, the particle concentration at 71 nm decreased to 0.8×10^6 parts / cm^3 due to the electrostatic precipitation effect. However, particle concentration for the particle diameter less than 20 nm did not increase.

It is known that fine particles are generated by ion-induced nucleation when corona discharge is generated in the gas included SO_2. Analysis of the components in the exhaust gas revealed that the SO_2 concentration in the exhaust gas using residual fuel oil was 37 ppm, although it was 2 ppm in the case of light fuel oil. Therefore, the increase the concentration for particles diameter less than 20 nm in the exhaust gas using residual fuel oil was due to ion-induced nucleation.

However, the total number collection efficiency in the exhaust gas using the residual fuel oil was 87%, and the ion-induced nucleation did not influent on the total collection efficiency. It is also known that the collection efficiency of fine particles can be improved by increasing the collection electrode length.

7CB.20

Sizing Sub-10 nm Particles from Engine Emissions. JOONAS VANHANEN, Jenni Alanen, Kati Lehtoranta, Sanna Saarikoski, Minna Väkevä, Topi Rönkkö, *Airmodus Ltd.*

It has been shown that a big fraction of the particle number concentration of an engine emission can be in sub – 10 nm size range (Rönkkö et al. 2017). The measurements conducted by Alanen et al. (2015) have indicated that some of these particles have a solid core as small as 2 nm in diameter. In this study, we measured nanoparticle number concentration and mean diameter from a natural gas engine using a modified Airmodus A20 butanol Condensation Particle Counter. In our measurements the particle mean sizes from engine emission were often between 3-6 nm. The mean diameters measured with the modified A20 bCPC agreed with mean particle diameters from SMPS measurement.

The A20 is a laminar, one flow instrument that has 5 nm lower cut-point with factory settings of 1 lpm flow rate, 39oC saturator temperature and 15oC condenser temperature. We have increased the flow rate up to 2.2 lpm, the saturator temperature up to 44oC and lowered the condenser temperature down to 10oC. The increase of flow rate lowers the diffusional losses especially for the smallest particles and the higher temperature difference between the saturator and the condenser increases the highest supersaturation for the n-butanol vapor inside the instrument. This makes it possible to activate and grow smaller particles with smaller losses. The grown particles are detected using light scattering. Every particle creates a pulse that is, in some extent relative to the initial size of the sampled particle (Marti et al. 1996). Smaller particles activate later inside the instrument than the bigger ones and thus have less time to grow. This creates smaller droplets and smaller measured pulses. The instrument was calibrated using silver nanoparticles in the size range of 2.3 nm to 40 nm. The 50% cut-off for silver particles was 3.1 nm, but the instrument was still capable of counting 20% of the 2.3 nm. Airmodus A20 measures the mean pulse width of the optical pulse created by the grown particle inside the CPC within the sampling time of 1 second. It was found that this mean pulse width corresponds nicely with the sample particle size from 3 to 10 nm. If there is no significant signal from particles larger than 10 nm, this information can be used to measure mean size of particles. This new method of using the mean pulse width enables the measurement of particle size and concentration with 1 Hz sample rate. Other instruments capable of measuring size distributions down to 3 nm usually have sample rate of a couple of minutes. In the future this method will be developed further to include full pulse width spectra for aerosol size distribution measurements.

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7CC.1

Hygroscopicity Measurements near Cloud Indicate Aerosol-Cloud Processing without Interrupting Ambient Measurements. STEPHEN NOBLE, James Hudson, *Desert Research Institute*

Transformations of atmospheric aerosols occur through processes within clouds. Clouds process aerosols in three ways; aqueous oxidation of trace gases within the droplets that add soluble material (chemical); collision and coalescence of droplets to combine soluble material from the aerosol (physical); and Brownian capture of interstitial particles to add soluble or less soluble material (physical). As most droplets evaporate, this leaves an altered particle from the one initially activated. This resulting particle is larger and more easily activates at lower supersaturations in subsequent cloud cycles. This activation improvement impacts cloud droplet number and size, and drizzle amount (Hudson et al., 2015; Hudson et al., 2018), which have implications for climate. Aerosol-cloud processing separates the processed (accumulation mode) and unprocessed (Aitken mode) aerosol. The resulting bimodal distributions have been observed in particle size measurements (Hoppel et al., 1986) and cloud condensation nuclei (CCN) measurements (Hudson et al., 2015). Hygroscopicity (κ) can be determined from particle size and CCN distributions, measured by critical supersaturation. Overlaying particle size and CCN distributions and tuning the κ value to produce agreement gives κ for the distribution. Separate tuning for Aitken (unprocessed) and accumulation (processed) modes provides κ for each mode. Differences in processing type are highlighted by κ differences between the two modes. Two aircraft field projects; a polluted stratus cloud study (MArine Stratus/stratocumulus Experiment, MASE), and a clean summertime cumulus cloud study (Ice in Cloud Experiment-Tropical, ICE-T); provide κ of the two modes. Differential mobility analyzers measured particle size distributions while the Desert Research Institute CCN spectrometer measured CCN distributions in both projects. In ICE-T, 60% of bimodal distributions had the same κ for both modes while in MASE only 26% had the same κ. This indicates collision and coalescence dominating in ICE-T where CCN with similar κ were combined through droplet coalescence. However, in MASE chemical processing via aqueous oxidation dominated because the two modes had different κ for 74% of bimodal distributions. This is consistent with Hudson et al. (2015). Generally, adding hygroscopic material through cloud processing makes processed κ greater than unprocessed κ. However, even when unprocessed κ is high, aqueous oxidation adds material that is less soluble (sulfates added to sea salts) and the resulting processed κ tends towards κ of the added material. This was evident in MASE. Cloud types in these projects appear to affect cloud processing type where larger vertical motions (W) in cumulus clouds create larger droplets that coalesce, while shallow stratus clouds with limited W promote chemical processing. More investigations among cloud types are needed. Here, the evidence suggests both types of processing existed to some extent in both projects. This new method to determine hygroscopicity is continuous; i.e., no interruptions of ambient particle size or CCN measurements; but may not be as exact as other methods. But, this κ measurement allows for investigation of aerosol evolution due to these natural cloud processes while providing information about relative particle hygroscopicity and can be performed after measurements have already been taken; i.e., used on archived data.

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7CC.2

Ccn Characteristics Observed at a High Altitude Site in Western Ghats. ARSHITHA ANAND K.A., R.S. Maheskumar, *Banaras HIndu University.*

Atmospheric aerosols which serve as cloud condensation nuclei (CCN) are key elements of hydrological cycle and climate change. In the present work, monthly and seasonal variation of CCN characteristics have been studied at Mahabaleshwar (1348 m AMSL) site in Western Ghats, using one year (December 2014- October 2015) of observations.

The study has been done in two sections first, we have seen how the CCN concentration varies with different supersaturation for different months and seasons during both daytime and nighttime separately. Later monthly and seasonal behavior of diurnal variation of CCN has been studied. CCN concentration shows higher values during both daytime and nighttime. Considering daytime and nighttime separately the monsoon season shows higher concentration during daytime and pre-monsoon shows higher concentration during nighttime. During the winter season, the Anthropogenic aerosols are dominant and due to calm wind during pre-monsoon and winter, the particles are less dispersive so it will be mainly confined to small area covering the study region. The seasonal dust is one the other reason for the increase in CCN concentration during pre-monsoon season. In the monsoon, the CCN concentration shows higher values because of the long range transport from the Arabian sea due to strong south-westernly wind. This result suggest that CCN concentration can be increased because of the emission of the aerosol particle from natural source such as forest, and also it can be increased because of anthropogenic activities. Overall analysis showed that CCN concentration was higher over this high altitude site despite of dominant sink process such as cloud scavenging and washout mechanism indicating local emission.

7CC.3

CCN Activity and Particle Growth of Aging Diesel Exhaust Particles. Humphrey Chukwuto, FRANK BOWMAN, *University of North Dakota*

Diesel exhaust particles emitted into the atmosphere undergo aging that changes their physical and chemical properties, but these processes are complex and not well understood. Laboratory chamber experiments were conducted to investigate the aging of diesel exhaust in the presence of UV light, ammonium sulfate particles, and/or α-pinene vapors. Particle growth and changes in number concentration and size distribution were monitored with a SMPS. Changes in CCN activity were measured with a CCN counter. Results from dark experiments with diesel exhaust alone showed no significant secondary organic aerosol formation and diesel exhaust particles that remained CCN inactive. Aging experiments with UV radiation resulted in a significant increase in particle mass, with deposition-corrected particle mass after 4 hours that was 20-60% higher than the initial mass of freshly emitted diesel soot particles. CCN activity also increased over time indicating that photooxidation of diesel exhaust vapors produces SOA more hygroscopic than the freshly emitted diesel particles. The addition of α-pinene to diesel exhaust in UV aging experiments further enhanced both CCN activity and SOA formation. Experiments with ammonium sulfate particles showed no discernible effect on SOA formation for either diesel exhaust alone or diesel exhaust/α-pinene mixtures. CCN activity measurements were consistent with a largely external mixture of hygroscopic ammonium sulfate particles and non-hygroscopic diesel soot, coated with moderately hygroscopic SOA. The results from this study underscore the importance of aging via photooxidation of SOA precursors and mixing with water-soluble particles in transforming hydrophobic soot into more CCN-active particles.

7CC.4

Characteristics of Cloud Condensation Nuclei in an Urban Region of Central Taiwan. TA-CHIH HSIAO, Wei-Jen Hsieh, Neng-Huei Lin, Chun-Chiang Kuo, *National Central University*

Cloud condensation nuclei (CCN) constitute a crucial fraction of atmospheric aerosols (Burkart et al., 2011). The physical and chemical characteristics of CCN is closely related to cloud development and precipitation process (Andreae and Rosenfeld, 2008). In urban region, traffic emissions, containing fresh small particles and hydrophobic substance, could be the major source for local air pollutions (Souto-Oliveira et al., 2016) and influencing the aerosols hygroscopicity and CCN's characteristics. Moreover, as aerosols released to atmospheric environment, different "aging processes", such as condensation, coagulation and oxidation, would change its physiochemical properties and enhance homogeneity as well as hygroscopicity of particles (Gunthe et al., 2011).

In this study, CCN's characteristics in Taichung city, which is the major metropolitan region in central Taiwan, was quantified by the activation ratio (AR = CCN number concentration/condensation nuclei concentration) during Sept. 2017 to Feb. 2018. The experimental hygroscopicity, κexp, proposed by Petters and Kreidenweis (2007) under the scheme of Köhler theory was further derived using AR and collocated particle size distribution (PSD) measurements. On the other hand, κchem was estimated based on the real-time aerosol chemical compositions, which were monitored by a PILS-IC system. The analysis between AR, particle size and hygroscopicity revealed two distinct groups of CCN characteristics in central Taiwan. One demonstrated a positive correlation with particle size and AR, and the other presented a relatively weak correlation. This suggests particle size and its chemical composition could both play important roles in aerosol's hygroscopicity and CCN's activity. Our data also show that κchem and AR is a function of wind direction (WD) and wind speed (WS), generally with higher values associated with winds from the south. The potential source contribution function (PSCF) analysis is further employed to investigate the contributions of potential local emission sources.

7CC.5

Large Indirect Radiative Effects of Smoke in the South-east Atlantic. HAMISH GORDON, Paul Field, Ken Carslaw, *University of Leeds*

Smoke from African fires mixes into clouds near Ascension Island in the south-east Atlantic, substantially influencing their radiative properties over a vast swathe of ocean[1]. The area of mixing coincides with the transition from stratocumulus to cumulus clouds, so any effects of aerosols on cloud cover are likely to be particularly important[2].

The clouds are strongly influenced by droplet concentration and liquid water path, both of which are difficult to represent in models. The droplet concentration requires accurate horizontal and vertical positioning of realistic aerosol plumes. In regional or global models, the liquid water path depends on correct representation of the boundary layer and on the sub-grid cloud fraction. Evaluation of the droplet concentration can be challenging as satellite retrievals may be compromised by above-cloud aerosol, which itself affects the properties of the clouds[3]. However, the recent CLARIFY campaign provides key in-situ data and fresh insights on how to deal with these issues.

This presentation will show how the aerosol-cloud interactions in this region can be represented in a convection-permitting regional Unified Model simulation driven by the HadGEM-UKCA global aerosol-climate model. The 4km-resolution regional simulation has two-moment aerosol driving two-moment cloud microphysics (the CASIM scheme[4]). In our model, the presence of smoke aerosol leads to a substantial increase in cloud droplet number, and also to significant effects on the cloud microphysics and boundary layer dynamics. We will highlight key challenges in simulating the stratocumulus-to-cumulus transition in the tropical Atlantic with large-scale models, for example the representation of aerosol mixing into the boundary layer. We will also show comparisons of our model to measurement data from the CLARIFY campaign.

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7CC.6

Cloud Effects on the Aitken and Accumulation Modes. JAMES HUDSON, Stephen Noble, *Desert Research Institute*

At SGP correlation coefficients, R, between remotely-sensed cloud fraction, cf, and time-lagged surface aerosol mean diameter (md) increased from zero (simultaneity) to maxima for aerosol ~five hours after cf. Delay was due to transit from cloud altitudes to surface. Peak Rs were greater for instruments with greater sky coverage (pyranometer gridded network [PGN]; total sky imager [TSI]) than ceilometer. But TSI and PGN operated only during daylight. Ceilometer cf-md Rs were also positive during daylight but negative at night. All three instrument peak Rs were also positive for cf-Aitken (< 100 nm; R = 0.54, 0.60 and 0.65; two-tailed probabilities, P2 < 10^{-8} for ceilometer [daylight], TSI and PGN, respectively) and accumulation mode md (> 100 nm; R = 0.27, 0.42 and 0.38; P2 4×10^{-5}, < 10^{-8}, < 10^{-8}, respectively). Negative peak Rs for cf-Aitken concentration were -0.30, -0.36, -0.35; P2 = 2×10^{-6}, < 10^{-8}, < 10^{-8}, respectively. Positive peak Rs for cf-accumulation concentrations were 0.23, 0.34, 0.34; P2 4×10^{-4}, 3×10^{-8}, 3×10^{-8}, for ceilometer, TSI and PGN, respectively.

Lagged md responses to cf > median cf steadily increased for ~five hours whereas lagged md responses to cf < median cf steadily decreased by similar md for ~five hours. When this was analyzed for consecutive hours of cloudiness or clearness, peak md increased/decreased by greater amounts.

More accumulation mode particles with larger sizes for greater cloudiness is consistent with aqueous oxidation, coalescence and Brownian scavenging by cloud droplets. These cloud processes thus account for the positive 0.47 R (P2 < 10^{-8}) between accumulation mode concentrations and sizes.

Negative Rs for cf-Aitken concentrations indicate more photochemical production for less cloudiness. Positive cf-Aitken size Rs indicate that initial photochemical particles are small. Brownian capture of cloud-interstitial particles also reduces Aitken concentrations, especially smaller Aitken particles because of their greater Brownian motion. This increases sizes of remaining Aitkens. Many Aitkens are converted to accumulation particles. The sizes of some larger Aitken particles are also increased by aqueous chemistry on those that nucleated cloud droplets. All of these processes make the negative R for Aitken concentration versus size (R = -0.42, P2 < 10^{-8}).

Separating Aitken concentrations by each hour of the day and according to above or below mean cf, all three instruments (six plots) show similar concentrations (~2000 cm^{-3}) for the first daylight hours. But after 10 AM concentrations increase by a factor of three for all plots except PGN cf > median cf, which remains below 2000 cm^{-3} all day. For cases when all three instruments simultaneously report cf > median cf, Aitken concentrations remained below 2000 cm^{-3} all day. The smaller numbers of cases when ceilometer or TSI cf > median cf but PGN cf < median cf cause the high midday ceilometer and TSI Aitken concentrations for cf > median cf. The consistently low PGN cf > median cf Aitken concentrations indicate that PGN greater sky coverage better represents the cloud conditions that inhibit photochemical Aitken particle production. The more local TSI and ceilometer sky coverages, therefore, misrepresent conditions most favorable for photochemical Aitken particle production.

Six similar hourly plots of accumulation mode concentrations also divided according to median cf are nearly identical for the three instruments; i.e., low accumulation mode concentrations for low cf throughout the day and factor of two higher concentrations for high cf with early afternoon peaks. Thus, the accumulation mode responds more to local cloudiness whereas the Aitken mode responds to more widespread clear skies.

7CC.7

Cloud and Aerosol Optical Analysis for Temperate Zona. Ibtissam Marsli, MOHAMMED DIOURI, Djamaleddine Chaabane, *Atmospheric Physic, LME, University of Oujda, Morocco*

Cloud and aerosol are of high importance in understanding the variability of radiative balance; they can also clarify the atmospheric evolution and remove the still significant uncertainties in climate change models. From the AERONET/PHOTONS network the data processing of about thirty sites distributed over the temperate zone allowed a precise characterization of the optical properties of clouds (optical thicknesses and occurrence frequencies) and aerosols (PSDs, single scattering albedo, optical depths and radiative forcing). This study concerns the analysis of data of the following sites: Maryland (38.99 °N, 76.83 °W), ARM_Graciosa (39.09°N, 28.02°W), La_Laguna (28.48°N, 16.32°W), Carpentras (44.08 °N,5.05°E), Weizmann_Institute (31.90°N, 34.81°E) , CEILAP-RG(51.60°S, 69.32°W) and Durban_UKZN(29.81°S, 30.94 °E). These seven sites are a sample representing the temperate zone from 77°W to 35 °E.

The histograms of the occurrence frequencies of the cloud optical depths reveal the dominance, as in the equatorial zone, and of identical way, of those included between 20 and 100 relating to low clouds as Stratus and Altostratus with 57%. For values below 20, the histograms are different and the appearance is dependent on the weather conditions of the considered region. The seasonal average of aerosol PSD show larger amplitudes with a maximum total volume concentration of 110, 58 10-3 (µm3/µm2) observed in Southeast of Mediterranean Sea. The corresponding accumulation and coarse modes determined for all the sites show median radii near 0.17 and 2.56 µm respectively.

The spectral time series (0.87 and 0.44µm) of the aerosol single scattering albedo appear to be relatively similar and vary on average between 0.6 and 0.98; this variability can be explain by the meteorological conditions of each region and local air pollution. The aerosol radiative forcing shows a tendency towards low local cooling, with annual average values near -125 W/m2 at the bottom and -15 W/m2 at the top of the atmosphere. The monthly averages of aerosol optical depth at 0.5 µm shows that the highest values are often record on summer with a maximum reaching 0.4. As on Equatorial area, the time series of the occurrence frequencies of the aerosol optical depths and those of the clouds indicate certain links to be confirm by a statistical approach, which requires a long-term monitoring.

7CC.8

Presence of Photosynthetic Microorganisms in Clouds. KEVIN DILLON, Pierre Amato, Martine Sancelme, Valdis Krumins, Anne Marie Delort, Donna Fennell, *Rutgers, The State University of New Jersey*

Clouds contain diverse microbial assemblages. Previous work has demonstrated that some heterotrophic microorganisms are active in clouds and have an impact upon cloud water chemistry. Photosynthetic microorganisms (cyanobacteria and algae) were also shown to be present. However, their diversity and activity as primary producers, i.e. as CO_2-fixing organisms, is still poorly characterized in clouds. To date, no photosynthetic isolates from clouds have been reported. Cloud water was collected at the puy de Dôme meteorological station (1465 m, France) and used to establish photosynthetic enrichments. Enrichments were initially incubated at 20°C. Once the enrichments were established, they were grown at ≈22°C, 15°C, and 4°C under 75 µE m^{-2} s^{-1} of light. These phototrophic microorganisms had a higher growth rate at 15°C, a relevant temperature for clouds, thus demonstrating the possibility that these are active in clouds. This is the first reported culturing of photosynthetic microorganisms from clouds. Current work is underway to obtain axenic photosynthetic cultures and to evaluate the diversity and activity of photosynthetic microorganisms in the atmosphere.

7CC.9

Hazardous Ice Cloud Avoidance Using Airborne LiDAR Remote Sensors. RICHARD STONE, Justin Fisher, *Sigma Space Corporation*

One particularly costly problem confronting manned and unmanned aircraft operations is icing. Current systems today can only detect icing once an aircraft is in cloud. These methods also do not provide sufficient information about large supercooled water droplets >50 µm) that jeopardize flight by “bleeding” back from the leading contact edges and freeze on the wings and airframe. Better measurements of cloud characteristics and identification of icing potential using remote sensing techniques can reduce icing hazards and threats before an aircraft encounters icing.

RHS Consulting operates an aircraft equipped with a side-looking radiometer (Radiometrics), a Mini Micro Pulse LiDAR (Sigma Space Corporation), and a cloud droplet measurement system (Droplet Measurement Technologies). This plane routinely flies in icing conditions and is being used to investigate winter storm systems by collecting data from each of these systems to investigate instrument performance.

Recent data from these flights shows that Micro Pulse LiDAR measurements by themselves, are sensitive to supercooled liquid and mixed phase clouds at distances up to 10 km, and offer the advantage of direct range observations that do not require ancillary data sets to produce cloud liquid water contents. They also offer the high potential to directly measure hydrometeor particle size distributions. Thus the Micro Pulsed LiDAR technique offers great potential for providing a small low cost solution for detecting icing hazards in supercooled liquid water and mixed phase clouds at distances up to 10km or more. Measurements from the latest flights will be presented and discussed.

7CC.10

The Cloud Feedback on the Heating Rate of Black Carbon and Brown Carbon. FERRERO LUCA, Grisa Mocnik, Gregorič Asta, Cogliati Sergio, Colombo Roberto, Rizzi Cristiana, Di Liberto Luca, Barnaba Francesca, Gobbi Gian Paolo, Bolzacchini Ezio, *GEMMA Centre, DISAT, University of Milano-Bicocca*

Black carbon (BC) and Brown Carbon (BrC) absorb sunlight and heat the atmosphere[1]. The heating rate (*HR*) can be determined from the divergence of the net radiative flux with altitude (vertical profiles) or from the modelling activity; however, its determination is, up to now, too sparse. Moreover, it does not account for light-absorbing-aerosol (LAA) speciation and for the influence of different sky conditions in the atmospheric layer below clouds[2,3]. This work applies a new method[4] to experimentally determine (at high time resolution) the *HR* induced by LAA in a atmospheric layer. Highly-time resolved measurements of *HR* were apportioned in the context of LAA species (BC, BrC), sources (fossil fuel, FF; biomass burning, BB)[5], and as a function of cloudiness.

Multi-wavelength aerosol absorption measurements were coupled with spectral measurements of the direct, diffuse and surface reflected radiation using: 1) Aethalometer (AE-31, Magee Scientific, 7-λ), 2) Multiplexer-Radiometer-Irradiometer (diffuse, direct and reflected radiance: 350-1000 nm in 3648 spectral bands), 3) a meteorological station (LSI-Lastem) including a full set of radiometers, 4) Lidar Ceilometer (CHM 15k „NIMBUS“ was used for the determination of cloud base height and its vertical depth; www.alice-net.eu), 5) condensation and optical particle counters (TSI 3775 and Grimm 1.107), 6) low volume sampler (FAI Hydra, $PM_{2.5}$ and PM_{10}).

To understand the importance of sky condition on direct, diffuse and reflected component of *HR* (HR_{dir}, HR_{dif}, HR_{ref}) the fraction of sky covered by clouds (oktas)[6] and the cloud type were considered. Cloud types were classified based on radiometric, spectroradiometric and lidar measurements[7] into several classes in function of cloud base height: 1) low level (<2 km) stratus, cumulus and stratocumulus; 2) mid level (2-7 km) altostratus, altocumulus; 3) high level (> 7 km) cirrus, cirrocumulus-cirrostratus; 4) clear sky conditions.

More than one year of 5 min data (March 2015 - November 2016) of *HR* were collected in Milan (Po Valley). The *HR* showed a clear seasonal behavior (winter: 1.83±0.02 K day^{-1}; summer: 1.04±0.01 K day^{-1}) with a daily cycle characterized by higher values in the morning (than in the afternoon) following the BC-BrC concentrations. On average (one year) the BC accounted for 1.05±0.02 K day^{-1} while the remaining 0.15±0.01 K day^{-1} was due to BrC.

Most important, the *HR* varied in different sky conditions, from 1.75±0.03 K day^{-1} in clear sky to 0.43±0.01 K day^{-1} in complete overcast (annual averages). Also the kind of radiation involved in the *HR* varied with sky conditions. For example, in clear sky conditions HR_{dir} was higher than HR_{dif} and HR_{ref} accounting on average for the 55±5% of total HR and leading alone to a HR_{dir} of 0.49±0.01 K day^{-1} in summer and of 2.04±0.03 K day^{-1} in winter. In cloudy conditions the only efficient component was HR_{dif} (82±1% of total *HR*; from 0.28±0.01 K day^{-1} in autumn to 0.49±0.01 K day^{-1} in winter). Thus, clouds have a very important feedback also on the aerosol direct radiative effect.

Cloud types were investigated also considering their effect on radiation spectrum striking on LAA characterized by different absorption Angstrom Exponent (AAE of BrC and BC). Particularly, both clear sky and cirrus conditions showed an impinging spectrum of diffuse radiation peaking in the blue region exerting a highly efficient interaction with BrC (with an average AAE of 3.66±0.03).

Thus, in clear sky and cirrus conditions the HR_{BrC} accounted for 11.4±0.6% of the total *HR* while this percentage decreased just to 2.8±0.8% in cloudy cases, as stratus, cumulus, stratocumulus, altostratus, altocumulus. To investigate the role of clouds, the variability of *HR* due to the radiation was decoupled from that due to LAA concentrations by normalizing it for unit mass of BC. Results showed the strongest impact on *HR* by low level cumulus clouds, which (according to lidar data) form on the top of the mixing layer in late spring.

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7CC.11

Characterization of Phase Changes in Clouds Using Hyper-spectral LIF-LIDAR. OFIR SHOSHANIM, Adva Baratz, *Israel Institute for Biological Research (IIBR)*

Cloud physics have great influence on global climate and Earth's energy budgets, however their empirical research is of great challenge. The dynamics of the formation and disappearance of droplets is governed by a critical thermodynamic balancing between atmospheric composition and its micro-meteorology. When raindrops are formed under such conditions, while falling through the atmospheric boundary layer, a cleaning air might occur due to droplet-aerosol coalescence. Since research in situ is the only way to fully conserve the atmospheric condition and thermodynamics, the optimal way to interrogate such processes in the atmosphere is by remote sensing.

The research presented here makes use of a fluorescent amino-acid molecule (Tryptophan) as a nuclei-bio-marker to interrogate the phase of a cloud. Its spectral signature in dry- or wet- form, allows to follow the phase changes and dynamics of the cloud using laser induced fluorescence LIDAR (LIF-LIDAR)[1]. The sensitivity to the spectral shifts and the anisotropy of the material's fluorescence is achieved in this work by exploiting the benefits of the hyper-spectral LIF-LIDAR which is based on an intensifier CCD (ICCD) sensor in a non-conventional way. We utilize this hyper-spectral LIF-LIDAR to measure the fluorescence spectra of aerosols (1-20 µm) from a distance of ~160 meters away. The back fluorescence from the aerosol phase is followed by UV photo-excitation (4th order of Nd$^+$YAG laser-266 nm) and detected simultaneously for both VV & VH polarization components. We also develop a technique of photon counting, which has been implemented on a full chip-image, to reduce the noise to signal ratio in the ICCD readout. The experimental setup includes a 3 sqrm aerosol-cell which is instantaneously controlled and monitored, following the fluorescence anisotropy, the elastic depolarization backscatter, the peak pulse power (pre- and post-cell), the generation and size classification of the aerosol phase, and the ambient conditions inside the cell.

This study demonstrates gradual vanishing process of the spectral Stokes shift due to the drying process of the Tryptophan aerosol inside the cell. This drying is also responsible for the increase in the fluorescence anisotropy of the suspended Tryptophan molecules. The research shows that remote sensing with hyper-spectral detection allows tracking phase changes of aerosols in the atmosphere. Such LIF-LIDAR setup increases the spectral perceptivity of aerosol remote sensing and demonstrate a novel technique to the study of cloud dynamics.

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7CC.13

Aerosol-Cloud Measurements during the NASA NAAMES Campaign: Summary of Data and Cloud Droplet Sensitivities.

RICHARD MOORE, Ewan Crosbie, Luke Ziemba, Mary Kacarab, Athanasios Nenes, Gao Chen, Johnathan Hair, Chris Hostetler, Claire Robinson, Michael Shook, Kenneth Thornhill, Edward Winstead, Bruce Anderson, *NASA*

We present a compiled dataset of airborne in situ measurements of aerosol and cloud microphysical properties and cloud condensation nuclei (CCN) spectra carried out during 2015-2018 as part of the 5-year North Atlantic Aerosols and Marine Ecosystems Study (NAAMES). These field campaigns target distinct cycles in the atmosphere above the annually-occurring North Atlantic phytoplankton bloom, which provide excellent opportunities to examine the influence of biogenic aerosols on CCN and clouds against a backdrop of both the presence and absence of anthropogenic pollution. Aerosol and cloud droplet number concentrations observed during November, 2015, were extremely low, while the addition of aerosol (by ~10- fold) during the Springtime increases cloud droplet number concentrations substantially. Results obtained during Fall 2017 are similar to those obtained in Spring 2016 in terms of mean aerosol loading. Meanwhile, the shape of the CCN supersaturation spectrum remains similar across all three deployments. In addition, we report the cloud droplet sensitivity to aerosol number, hygroscopicity, and cloud updraft velocity. The results of NAAMES and sensitivity of cloud droplet number to aerosol loading will be contextualized within the results of past airborne campaign targeting aerosol-cloud interactions.

7CC.14

New Particle Formation Impacting Cloud Condensation Nuclei Concentration. ANNA GANNET HALLAR, Lauren Zuromski, Ian McCubbin, Douglas Lowenthal, *University of Utah*

There are several potential underlying principles that allow aerosol nucleation to occur more frequently at high elevation sites. Previous work has shown that frequent New Particle Formation (NPF) occurs regularly (52% of days) at a remote high elevation (3210 m a.s.l.) site in Colorado, Storm Peak Laboratory (e.g., Hallar et al., 2011; Hallar et al., 2016). This new work will present a long-term climatology (2001 – 2017) of aerosol size distributions and clearly shows a seasonal dependence on new particle formation at Storm Peak Laboratory. Furthermore, using this extensive data record, an aim of this study is to demonstrate a statistically significant connection between NPF events and growth to Cloud Condensation Nuclei (CCN). Ambient CCN data Storm Peak Laboratory has been collected for the last decade. These new results suggest that NPF in this remote region are directly impacting the number of available CCN at a supersaturation relevant to orographic cloud formation.

7CD.1

Oxidative Potential of Ambient Aerosols: First Measurement over Santiago Metropolitan Area. Carolona Molina, Vishal Verma, Victor Vargas, LEIVA G. MANUEL A., *Facultad de Ciencias, Universidad de Chile*

In Chile, almost 90% of the population lives in polluted urban areas, such as Santiago Metropolitan Area (SMA, 33.5ºS, 70.5ºW), the capital of Chile. In SMA, the levels of PM often exceed national air quality standards and guidelines of the World Health Organization. The exceedance of limit values for both PM10 and $PM_{2.5}$ occurs mainly due to urban expansion, domestic heating, growth of diesel vehicles fleet, and industrial activity. The particular geographic and meteorological conditions in SMA have additional effects on air quality. The population of SMA (7 millions inhabitants) are exposed to high levels of air pollution.

It is shown that PM produces adverse effects on human health, even at low concentrations. Although the mechanisms of PM related health effects are not well understood, the most accepted hypothesis considers the PM-induce inflammatory processes by promotion of oxidative stress; as a result of over-generating reactive oxygen species (ROS) and radical species that exceed the available antioxidant defenses producing cell damage. Therefore, the oxidative potential of PM (defined as a measure of the capacity of PM to oxidize target molecules and generating ROS or other reactive species) is a good indicator of its toxicity. Despite its importance, the oxidative potential of PM has not yet been studied over SMA, as per our knowledge.

In the present work, a dithiothreitol (DTT) assay was used to measure the ROS-generation potential of water-soluble $PM_{2.5}$ and PM_{10} of 30 ambient PM samples. The results obtained show that even when the mass proportion of PM2.5 over PM10 is around 60%, the proportion in OP is 80%; indicating that the highest loss activity of DTT is contributed mainly by the fine fraction of the PM in SMA. The comparison of OP values with other cities in the world shows that the OP of SMA ambient PM is at upper end of the typical range observed for ambient PM. Finally, these preliminary results show the importance of systematically measuring the OP of PM in SMA; and even more in other polluted cities of Chile where the PM mass concentrations exceed even SMA.

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7CD.2

Intranasal Airway Deposition of Dry Particles in Physical Models of Children and Adults during Inspiratory Flow Rates Representing Rest, Light, Moderate and Heavy Activity.

Jana Kesavan, VALERIE J. ALSTADT, Jerold Bottiger, Keith Sedberry, Beth Laube, *US ARMY ECBC*

Background: Although the potential for negative health effects from deposition of toxic particles in the intranasal airways of children makes determination of deposition in this region essential, studies of particle deposition that include exposing infants and children are not feasible. Anatomically-correct physical models provide a method for quantifying intranasal deposition of inhaled particles without direct exposure to humans. Toxic particles may be liquid or dry. However, little is known about intranasal deposition of dry particles during different activity levels within physical models of young children.

Methods: We used stereolithography and CT scans to generate anatomically-correct physical models of the head, face with nostrils and intranasal airways of a 2 and 5 year-old child and 18 year-old adult. We then quantified and compared deposition of 1-10 µm dry particles of Arizona Test Dust in the intranasal airways of the models during inspiration only, at flow rates representing rest, light, moderate and heavy activity. Data were standardized using the impaction parameter, so that deposition in the three models could be compared.

Results: Intranasal deposition of 2.458 µm dry particles at light activity flow rates was similar for all three models. However, deposition was significantly greater in the 2 and 5-year-old models, compared to the 18 year-old model, for particles smaller and larger than 2.458 µm, during inspiratory flow rates representing rest and light activity. Deposition in the 5 year-old was greater than in the 18 year-old for all particles ≥2.458 µm during moderate activity and ≤8.977 µm during heavy activity. Deposition in the 2 year-old model was significantly greater than in the 5 year-old model for ≥4.698 µm particles at light activity flows and for all particle sizes at moderate and heavy activity. Variability in intranasal deposition for the three models was reduced when standardized in terms of impaction parameter combined with the anatomical parameters of Amin (the minimum cross-sectional area of the nostrils) and Ellipticity (the ratio of nostril length to width).

Conclusions: Intranasal deposition of dry particles between 1-10 µm may be greater in 2 and 5 year-old children, at rest and during light activity, compared to adults, and may be greater in 2 year-old children, compared to 5 year-olds, during moderate and heavy activity. These results suggest that the intranasal airways of 2 and 5 year-old children may be at risk for detrimental health effects from increased exposure to toxic dry particles during nasal breathing, compared to adults. Studies in additional models based on similar age children are needed to confirm these findings.

7CD.4

Investigating the Effects of Cookstove Emissions on Ocular and Cancer Cells. BEDIA KARAKOCAK, Sameer Patel, Nathan Ravi, Pratim Biswas, *Washington University in St Louis*

2.7 billion people burn solid fuels for cooking and heating using stoves, with major health consequences. Solid fuel combustion emissions increase the prevalence of illnesses such as chronic obstructive pulmonary disease and lung cancer; however, their effect on eyes is underexplored. In this novel study, three healthy ocular cell lines (corneal, lens, and retinal epithelial cells) and a cancer cell line were exposed to gas and liquid phase combustion emissions from applewood and coal.

In the first part of the study, three healthy ocular cell lines underwent controlled exposures on three separate occasions to filtered air, applewood, and coal smoke from incomplete combustion for one hour in a controlled chamber. In the second part, particles formed as a result of biomass combustion were collected on a filter. The ocular and cancer cells were then exposed to the filter extracts for 24 hours.

The viability of the cell lines exposed to stove emissions was assessed by measuring real-time cell attachment behavior and cell metabolic activity. Reactive oxygen species (ROS) generation was also quantified. For both phases, the results indicated that coal emissions compromised the viability of ocular cells more than applewood emissions. Interestingly, the cancer cells, although their viability was not compromised, generated 1.7 to 2.7 times more ROS than healthy cells. This acute exposure study provides compelling proof that biomass combustion emissions compromise the viability of ocular cells and increase ROS generation. The increased ROS generation was fatal for ocular cells, but it promoted the growth of cancer cells.

7CD.5

Reactive Oxygen Species of Ambient Water-soluble PM2.5 in the North and Northwestern China: Contrasts in Concentration and Sources. YAQING ZHOU, Rujin Huang, Junji Cao, *Key Laboratory of Aerosol Chemistry and Physics, IEECAS*

$PM_{2.5}$ pose an unequivocally health problem, which may penetrate deeply into the human respiratory system and leading to oxidative stress. China has suffered severe haze problems during winter in recent years. So far, a direct causative link between particle properties and adverse health effects and the main sources of these toxic components is currently lacking. In this study, the ROS concentration, link between chemical components and ROS, source apportionment of particle-bound ROS are reported in three major cities in north and northwestern China. The average particle-bound ROS concentration in Beijing, Xi'an, Shijiazhuang during 2013 winter were measured using DCFH method, which were 0.43±0.38, 0.89±0.55 and 0.76±0.46 nmol $H_2O_2 \bullet m^{-3}$, respectively. The mass ROS efficiencies of three cities were 0.005, 0.005 and 0.002. Xi'an has the largest ROS concentration and mass efficiency. Different level of water-soluble metal seems to have obvious influence on ROS that high water-soluble Fe may accelerate the formation of ROS, and high water-soluble Cu may reduce the increase of ROS. Based on preliminary source apportionment result, vehicle emission has the largest contribution (40%) to ROS, and biomass burning increase obviously when air condition changed from cleans days to extreme pollution days.

7CD.6

A New Risk Grouping Concept for High Aspect Ratio Materials - The Fibre Dustiness Test by Vibro-Fluidization.

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Introduction High aspect ratio materials (HARM) like carbon nanotubes (CNT) exhibit material properties that enable innovative applications but also raised concerns about potentially harmful effects to humans due to their asbestos-like morphology. Control banding by grouping of HARM by hazard- and exposure-related properties is a promising approach to risk assessment and risk mitigation for a large family of materials. Such grouping requires identifying dust release quantifying properties that enable a differentiation of HARM with low, moderate or high dustiness together with information on dust morphology.

Methods We have developed a dustiness test for powdery HARM and studied it for a broad range of CNT materials. Fibre dustiness testing was performed by vibro-fluidization that passes a low-volume airflow through a vertically vibrating powder column. Vibration allows overcoming adhesive forces between powdery agglomerates that would otherwise hinder fluidization. The vibro-fluidization method allows controlling airflow, vibration amplitude and frequency. The released aerosol was monitored and collected downstream to study the dust generation process and to determine process and material-related parameters. All collected samples were analysed by means of scanning electron microscopy (SEM) to obtain detailed information on the dust composition and its morphology.

Results and Discussion We performed dustiness tests on 15 different types of MWCNTs. The results allowed to develop a material ranking scheme based on the emission propensity for different morphological dust classes and to define distinct emission bands for low, moderate and high dustiness. SEM-based morphological analysis, of more than 500 emitted objects per material, enabled us to rank HARM according to their propensity to emit fibres in individual or agglomerated form. We also measured pair-wise distributions of diameter and length to identify and quantify potentially rigid fibres and those matching the WHO definition for potentially hazardous fibre geometry with a self-developed software. The obtained results form the basis of our proposed new grouping strategy for control banding that classifies HARM using a risk matrix. The matrix considers both intrinsic material and process-related properties such as bio-durability, toxicity as well as dustiness, grade of agglomeration and presence of hazardous WHO-fibres.

7CD.7

Oxidative Potential of Ambient Fine Aerosol during Intense Biomass Burning over the Indo-Gangetic Plain-India. ANIL PATEL, Rangu Venkata Satish, Atinderpal Singh, Darshan Singh, Neeraj Rastogi, *Physical Research Laboratory, Ahmedabad, India*

Emissions from biomass burning (BB) are dominant global source for carbonaceous aerosol and gases in the atmosphere. On regional scale, the emission budget reveals that nearly 400 Gg of particulate organic carbon (OC) are produced per year from post-harvest paddy-residue burning emissions in the Indo-Gangetic Plain (IGP). Particulate matter (PM) from BB, mostly comprised of fine carbonaceous aerosol, may have significant impact on regional air quality and human health as they are capable of penetrating into the alveolar region and might absorbed into the blood stream of the human body that may cause various cardio-pulmonary diseases. A widely accepted proposed mechanism related to the effect of PM on human health is that inhaled ambient PM generates reactive oxygen species (ROS), which further cause cellular damage and induce oxidative stress in human. Capacity of PM to generate ROS is termed as their oxidative potential (OP). A variety of cellular and acellular assays have been developed to quantify different aspects of PM-induced oxidative stress based on the possible mechanistic route linking aerosol chemistry to health.

In present study, daytime and nighttime $PM_{2.5}$ (PM with aerodynamic diameter less than or equal to 2.5μm) samples (n = 69) were collected on tissuquartz filters using high volume air sampler during October–November, 2014 over a semi-urban site (Patiala: 30.2°N; 76.3°E, 250m amsl) in the IGP, India. In parallel, the mass concentration of black carbon (BC) was also determined with seven wavelengths Aethalometer. Study period covers the ambient air conditions of the study region before, during and after a large scale post-harvest paddy-residue burning to assess the effect of biomass burning emissions on the OP of aerosol. Filter samples were analyzed for major anions, cations, organic carbon (OC) and elemental carbon (EC), water soluble organic carbon (WSOC), sugars including levoglucosan, and trace metals. Further, a widely used dithiothreitol (DTT) assay was used to measure the OP of soluble ambient $PM_{2.5}$.

Volume normalized OP (OP m^{-3}) is found to be highly correlated ($R^2 \geq 0.70$, $p<0.05$) with many BB markers such as OC/EC, K^+/EC, BC_{370}/BC_{880}, and levoglucosan, which attests that observed OP is mainly due to species emitted from BB. OP m^{-3} exhibited a positive significant correlation with ambient $PM_{2.5}$ mass concentration during paddy-residue burning period ($m=0.037$, $R^2=0.78$, $p<0.05$) with ~ 2 times higher slope compared to that reported for winter (Jan-2014, $m=0.017$, $R^2=0.44$, $p<0.05$) from the same site. It is attributable to dominant contribution of species from BB to $PM_{2.5}$ during study period, which should have higher OP. However, mass normalized OP (OP μg^{-1}) was found to be increasing during post-burning period, which suggests that the aging and/or atmospheric processing of PM species from BB increase their OP. Further, OP μg^{-1} is found to be significantly correlated with ratio of WSOC to secondary inorganic aerosol (SIA) in daytime samples collected during paddy-residue burning ($m=25$, $R^2=0.59$, $p<0.05$, $N=16$) with ~ 5 times lower slope than that observed during winter 2014. WSOC during winter was reported to be predominantly of secondary origin whereas during this study, it was mixture of primary (from BB) and secondary sources. This observation suggests that WSOC formed through secondary processes are more DTT active than those emitted directly from primary sources. Such studies have implications in understanding the role of PM from BB emissions on air quality and atmospheric chemistry over a given study region, and designing appropriate mitigation strategies.

7CD.8

Identification of Toxicity Parameters Associated with Combustion Produced PM2.5 Surface Chemistry and Particle Structure by in Vitro Assays. RANDY VANDER WAL, Madhu Singh, Patricia Silveyra, Joshua Muscat, *The Pennsylvania State University*

Introduction: The International Agency for Research on Cancer (IARC) has labeled diesel exhaust as carcinogenic within class 1. While the mechanism(s) by which soot causes the adverse health effects are not known, a great deal of these harmful effects relate to its ability to cause oxidative stress. Thus, oxidative potential, expressed through reactive oxidative species concentration, can be used as a good estimate for its reactivity and toxicity. Accordingly, physical structure and surface chemistry become surrogate measures of its oxidative potential as together they determine the redox properties and polar/acidic character. Based on this premise, we are testing the role and impact of soot structure and surface chemistry upon interaction with bronchial and alveolar epithelial cells. The proposed project's goal is the identification of toxicity, oxidative, and pro-inflammatory factors in combustion produced soot arising from using alternative fuels, by studying the particles directly instead of studying compounds adsorbed on (and removed from) the soot particles. Model soots with tailored surface chemistry, and specific particle physical structures are being tested for toxicity, oxidative stress markers, effects of lung inflammation and and signaling pathways using cell culture bioassays, as well as protein carbonylation and DNA damage marker assessment.

Methods: An epithelial cell line (BEAS-2B) was incubated with lab-generated carbon (nascent, nitric acid-treated, and ozone-treated carbon) for 6 hr. and 24 hr. incubation times, at different concentrations (0-100 µg/mL). After incubation, we measured cell viability using the MultiTox-Fluor Multiplex Assay. In addition, we extracted RNA and protein from cells to evaluate expression of inflammatory cytokines (IL-1b, IL-6, IL-8) and genes related to the inflammatory response and oxidative stress (TLR4, CCL2, MMP1, and NRF2).

Results: Treatment of carbon particles with nitric acid and ozone resulted in differential oxygen and carboxylic acid content in the $PM_{2.5}$ surface. In BEAS-2B cells, an inverse relationship of cell viability and $PM_{2.5}$ treatment concentration was observed at both time points assessed. Of the three $PM_{2.5}$ preparations, BEAS-2B cells exposed to nitric acid-treated carbon resulted in the largest decrease (89% and 96%) of cell viability after 6 hr. and 24 hr., respectively, indicating that both carboxylic acid and oxygen content of the particle surface strongly contribute to $PM_{2.5}$ toxicity. Additional results showed an increase in gene expression of the inflammatory cytokines IL-1b, and IL-6, and the oxidative stress markers TLR4 and NRF2 at higher concentrations of PM2.5 exposure (25-100 µg/mL).

Conclusion: In summary, exposure of different types of particulate matter to lung epithelial cells increases inflammatory responses, with different effects associated with soot components such as particle surface chemistry. Future experiments will determine how functional groups in the $PM_{2.5}$ surface chemistry affect the activation of the observed inflammatory response, and decrease in cell viability of lung epithelial cells.

7CD.9

Near-Roadway Effects on the Progression of Alzheimer's Disease. KEITH BEIN, Christopher Wallis, Xiao-San Luo, Kelley Patten, Anthony Valenzuela, Elizabeth Berg, Jill Silverman, Pamela Lein, Anthony S. Wexler, *University of California Davis*

Recent epidemiological studies have linked traffic-related air pollution (TRAP) to increased risk of Alzheimer's disease (AD). In addition, in vivo and in vitro studies have shown that individual components of TRAP can alter neuroinflammation, increase neurotransmitter levels, and increase neurogenesis. However, TRAP exposures are challenging to reproduce in laboratory settings, and the mechanisms by which TRAP leads to Alzheimer's-related cognitive deficits remain unclear. To address these issues, we exposed male and female wildtype and transgenic Fischer 344 (TgF344-AD) rats to real-time TRAP, using an exposure facility that samples air directly from a highway tunnel in the Bay Area of California used by both light- and heavy-duty vehicles. TRAP and filtered air (FA) PM samples were collected for 24 hours once every third day, and a subset of these were analyzed for particulate matter mass, organic and elemental carbon composition, and elemental composition. Gas phase samples were collected monthly on sorbents and analyzed for molecular organics. The goal of this project is to test the hypotheses that exposure to TRAP triggers inflammatory responses in the brain that initiate, accelerate or exacerbate progressive AD pathology and cognitive dysfunction, and that the response to TRAP varies depending upon sex, age, and expression of AD susceptibility genes. To test these hypotheses, we are quantifying cytokines in the periphery and brain, neuroinflammation, neuropathology, and cognitive impairment in rats genetically predisposed to AD and their wildtype littermates exposed to TRAP or FA beginning at postnatal day 28.

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7CD.10

Evidence of Atmospheric Secondary Transformation of Transition Metals and Impact on Particle Oxidative Potential.

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Exposure to fine Particulate Matter (PM2.5) has been linked with various adverse health effects. Particle bound metals, especially transition metals, are hypothesized to initiate respiratory disease and trigger systemic inflammatory disease response. Understanding the role of metals in PM induced health effects is key to mitigate the impact of air pollution and protect public health. Iron is the most abundant PM transition metals from various sources including road dust, traffic, industrial and ship emissions. Many research studies have shown positive association between water soluble iron and the generation of reactive oxygen species (ROS) as the pathway to oxidative stress. However, the two different oxidation states of ferrous (Fe(II)) and ferric (Fe(III)) can be inter-converted in which photoreduction of Fe(III) to Fe(II) theoretically participates in a catalytic cycle to produce toxic hydroxyl radicals (·OH) and Fe(II) can also be oxidized to Fe(III) by molecular oxygen to generate superoxide anion O2- while Fe(III) plays an important role in various redox reactions. This study combines both real world field investigation to provide evidence-based knowledge on the particle bound water soluble iron speciation, and laboratory investigation to evaluate the impact of atmospheric processing and aging on the conversion between Fe (II) and Fe (III). Clear evidence was found in the atmospheric transformation of the transition metal of iron during day and evening times, same with the laboratory controlled UV exposure experiments. Controlled tests and spike tests with addition of ironic components showed their positive contribution to the overall oxidative potential of aerosols. The reactive oxygen species generated from the fresh and secondary formed aerosols also showed clear difference suggesting the strong impact of transformation of transition metals on the health implications. This study is one of the first investigations of its kind, and we expect the results will form the basis to better understand the relation between particle metals and health effects.

7CD.11

Generating Biodiesel and Fossil Diesel Exhaust Particles with Varied Physico-Chemical Properties for Toxicological Studies.

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Introduction

Diesel exhaust (DE) is classified as carcinogenic and is suspected to play an important role in the adverse effects of ambient PM in urban areas. Candidates for toxicologically relevant particle properties include the specific surface area and surface reactivity of the solid black carbon core, the liquid organic fraction including polycyclic aromatic hydrocarbons (PAHs), and transition metals.

The use of renewable fuels such as rapeseed methyl ester biodiesel (RME) and hydrotreated vegetable oil renewable diesel (HVO) in the commercial and private transport sectors is increasing. The fuels reduce net green house gas and alter health relevant emissions compared to fossil diesel (Murtonen et al., 2009). The largest reduction of emitted PM is attributed to RME, however its oxygenated organic fraction has been linked to increased oxidative potential and higher in-vitro toxicity (Hedayat et al., 2016). The chemical composition of HVO fuel is more similar to fossil diesel , so far the knowledge of its exhaust emissions is limited.

We here describe an approach where the particle composition and properties can be varied over a wider range and in a more systematic way compared to previous studies while maintaining realistic engine operation conditions. Exhaust, from a modern heavy-duty diesel engine fueled by fossil diesel, 100% RME and 100% HVO biodiesel , was characterized and collected to be used in a n in-vivo toxicological study.

Method

A six cylinder heavy-duty diesel engine modified for a single cylinder operation was used for the experiment. The engine was run at a fixed engine operating load with varying exhaust gas circulation (EGR). The exhaust gas was sampled after a partial flow dilution tunnel. Exhaust particles were characterized using real-time aerosol mass spectrometry (AMS), a fast mobility particle analyzer (model DMS 500), aethalometer (model AE33), thermal optical analyser (OC/EC) and Transmission Electron Microscopy (TEM). Toxicological studies require large amount of PM (~30 mg). A High Volume Cascade Impactor (HVCI 900, BGI Inc.) followed by methanol extraction and a Versatile Aerosol Concentration Enrichment System (VACES) was used to collect the particles.

Conclusion

EGR reduced the amount of O_2 and the temperature in the combustion cylinder (a common NO_x reduction strategy) . EGR also strongly affected PM emission levels and properties. PM with particle mass fractions ranged from: elemental carbon: 30-80%, organic carbon 20-70% and the PAH/org* fraction: 0.002 - 0.080. The particle size varied with fuel type from 79 (RME)–102 (diesel) nm. Low EGR affected the nucleation mode and CMD.

The collected particles were successfully extracted from the HVCI filters with an extraction efficiency of 85-105%. Currently, a pulmonary exposure study of these particles in mice is in preparation, together with detailed characterization of collected nano material including BET surface area analysis , Reactive Oxygen Species assays and a thorough TEM analysis of the soot micro- and nano structure. The aim of the in-vivo study is to identify relationships between particle physico-chemical properties and biomarkers of genotoxicty, inflammation and cardiovascular effects.

Acknowledgement

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7CD.12

Toxicity Testing in Human Airway Epithelial Cells for Particulate Emissions Resulting from Alternative Fuels. C.M. SABBIR AHMED, Jin Chen, Jiacheng Yang, Cody Cullen, Georgios Karavalakis, Ying-Hsuan Lin, *University of California, Riverside*

Traffic-related particulate matter (PM) has been associated with a broad range of adverse health effects in humans including respiratory, cardiovascular, cancer, central nervous system, developmental and reproductive health outcomes. Recently, alternative fuels have been widely used to reduce greenhouse gas emissions and oil imports. As fuel compositions change, there is a need to conduct systematic emission and toxicity testing to evaluate their potential impacts. In this study we assess the toxicological potency of PM emissions from a current technology vehicle equipped with a gasoline direct injection (GDI) engine when operating on eight different fuels with different compositions, including aromatic hydrocarbon contents, ethanol content, and PM index (PMI). Testing was conducted over the LA92 driving cycle using a chassis dynamometer. PM samples are extracted and examined using an in vitro model of human airway epithelial cells (BEAS-2B). Aerosol oxidative potential, XTT-based cell proliferation assays, the release of lactate dehydrogenase (LDH), and expression profiling of oxidative stress, inflammatory cytokines and metabolic syndrome related genes are assessed to determine the relative toxicity of PM resulting from various compositions of the fuels. Aliquots of the exhaust filter extracts are analyzed to determine the PM compositions at molecular level. The study will investigate associations among fuel compositions, physiochemical properties of PM, aerosol oxidative potential and PM-induced health effects to understand the potential health risks from alternative fuel formulations and GDI engines.

7CD.13

Reactive Oxygen Species Generation by Particle Size-dependent Transition Metal Ions using a Kinetic Multi-layer Model in the Epithelial Lining Fluid. TING FANG, Pascale Lakey, Rodney J. Weber, Manabu Shiraiwa, *University of California, Irvine*

Soluble transition metal ions (e.g. Fe and Cu) in particulate matter (PM) are critical aerosol species to generate reactive oxygen species (ROS) upon deposition in human respiratory lining fluid by redox cycling, Fenton, and Fenton-like reactions, leading to oxidative stress and adverse health effects. Quantifying ROS generation in respiratory system is important in understanding the health effects of particulate metals, but direct measurements of ROS in respiratory tract is so far not available. The kinetic multi-layer model of surface and bulk chemistry in the epithelial lining fluid (KM-SUB-ELF) [1] has been developed to estimate the amount of ROS generated within the ELF by simulating the reactions of transition metal ions with antioxidants. Particle sizes affect the location and amount of ambient soluble transition metal ions deposited in the respiratory system and thus affects the ROS generation. In this study, ambient size distribution of water-soluble transition metal ions were obtained by analyzing MOUDI (Micro-Orifice Uniform Deposit Impactor) samples collected from a road-side and representative urban site in Atlanta, GA. Deposition of transition metal ions in the ELF were then estimated using an empirical expressions derived from human inhalation data (ICRP) [2,3]. The KM-SUB-ELF model was then applied to the deposition data to estimate the size-dependent ROS generated in the ELF by transition metal ions in the nasal cavity, bronchi, and alveoli. We summarize and compare the ROS generation due to transition metal ions in different segments of human respiratory tract and compare to the reference level between healthy human and those with respiratory diseases.

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7CD.14

Spatial and Seasonal Patterns in the Oxidative Burden of Ambient Particulate Matter in Urban Centres. ALISON TRAUB, Cheol H. Jeong, Cuilian Fang, Maryam Shekarrizfard, Ryan Kulka, Hongyu You, Marianne Hatzopoulou, Scott Weichenthal, Greg J. Evans, *SOCAAR, University of Toronto*

Exposure to fine airborne particulate matter (PM) is associated with a broad suite of adverse health effects, including cardio-respiratory, neurological, and even metabolic disease (e.g., Alderete et al., 2017; Lim et al., 2012; Oudin et al., 2016). Although there is much uncertainty as to the mechanism of disease evolution following exposure to PM, a likely mechanism is cell and tissue damage as a result of oxidative stress and inflammation (Donaldson and Tran 2002; Li et al. 2003).

In light of this likely mechanism, oxidative potential (OP) – the ability of PM to cause oxidative stress, measured per unit mass of PM – and oxidative burden (OB) – the ability of PM to cause oxidative stress, measured per unit volume of air – have emerged as promising, biologically relevant metrics for assessing risk associated with atmospheric PM (Ayres et al. 2008). Unlike PM mass, these metrics are associated with both cellular inflammatory response, cause-specific mortality, and other adverse health effects (e.g., Harrison and Yin, 2000; Weichenthal et al., 2016).

Assessment of PM OB at high spatial resolution in urban centres could facilitate population-level epidemiological studies. These studies could help inform public policy by providing location-specific information about which PM components contribute most to toxicity in these densely populated areas. To achieve this goal, there is a need for data on ambient PM OB that has high spatial resolution, isolates temporal and spatial variability, and accounts for the effects of oxidation by all redox-active PM components.

This study examined the OB of ambient PM collected simultaneously from 80 sites across the city of Toronto, Canada's largest city with a population in exceedance of 5 million. To our knowledge, this study will have the highest spatial density of any PM OB study by at least an order of magnitude. Further, simultaneous sample collection for two-week periods in Summer 2016 and then Winter 2016-17, allows us to examine spatial and temporal variability separately.

A further goal of this study is to compare OB results using three different measurement techniques. Specifically, PM OB is being assessed using three common in vitro methods: the ascorbate (AA) assay, the glutathione (GSH) assay, and the dithiothreitol (DTT) assay. Previous studies have identified that these three assays are sensitive to different components of ambient PM (e.g., Calas et al. 2017; Fang et al. 2016; Weichenthal et al. 2016). Therefore, the combined use of these three common assays will provide a more comprehensive picture of PM OB and will help to elucidate the relationship between OB measurements made using these assays. Although analysis for Toronto samples is still underway, patterns suggest that the OB measured with the GSH assay exhibits both the greatest spatial variability and the strongest seasonal dependence, followed by the OB measured by the DTT and AA assays.

7CD.15

Non-additive Effects of the Mixture of Metals and Organic Compounds to Mammalian Cell Cytotoxicity of Particulate Matter (PM).

YIXIANG WANG, Michael Plewa, Vishal Verma, *University of Illinois at Urbana-Champaign*

The adverse health effects of particulate matter (PM), including the PM-catalyzed biological generation of reactive oxygen species (ROS), have been widely studied. Due to the complexity of PM chemical compositions, generally pure chemicals (e.g., standard organic and metals solutions) are studied to assess the toxic effect of PM components. However, the applicability of these methods to understand the interactions among the PM components has not been validated. To address these questions, we selected several metals (Cu, Fe, Mn) that are related to the oxidative potential (OP) of PM and assessed their interactions with the organic compounds in inducing the toxicity. Chinese Hamster Ovary (CHO) cells were used for assessing the cytotoxicity of the PM. Metals constitute one of the most toxic fractions of ambient PM. Our preliminary tests showed that after removing the metals from the PM matrix using Chelex column, the toxicity decreased from 90% to 20%. Therefore, an artificial metals mixture was prepared in the same concentration as the hydrophilic fraction (rich in metals) of the PM extract, but it expressed much lower toxicity than the PM samples, indicating some interaction of metals with the organic compounds for inducing the toxicity. We also plan to measure the OP of metals and PM samples in the same cytotoxicity level by dithiothreitol (DTT) consumption, and •OH generation in surrogate lung fluid (SLF) and DTT assays to investigate the differences of pure components and mixtures in ROS generation. Our study highlights the need to account for the interactions between organic compounds and metals while apportioning the relative contributions of chemical components in the PM toxicity.

7CD.16

Toxicity Evaluation of Secondary Organic Aerosol on Human Lung Cells. PRATITI HOME CHOWDHURY, Tanya Lasitza Male, Quanfu He, Michal Pardo, Yinon Rudich, *Weizmann Institute of Science*

Adverse health effects due to exposure to particulate matter (PM) are among the most important global environmental health risks. However, the effects of exposure to secondary organic aerosols (SOA), major component of the global aerosols, are largely unknown. To understand the effect of real environmental exposure on the respiratory system we simulated SOA from biogenic and anthropogenic sources mimicking day time ambient aerosol. In this study, we exposed lung epithelial cells (A549) to aged SOA particles (equivalent to 3 days) using air liquid interface (ALI) cell exposure system, thus mimicking the deposition of fine particles in the lung. SOA were generated using Oxidation Flow Reactor (OFR) that provides a highly oxidizing environment that simulates atmospheric oxidation processes under NOx-free and high NOx conditions. Both anthropogenic and biogenic volatile organic compounds (naphthalene and α-pinene, respectively) were used as the SOA precursors. Our preliminary results show a significant decrease in cell viability and significant increase in ROS when exposed to SOA in compared to clean air and incubator control. other parameters related to cell oxidative stress and inflammation were shown to vary after exposure to SOA. This study elucidates at least in part some of the biological responses of SOA and their biochemical pathway of toxicity.

7CD.17

Simultaneous Measurements of Lung Deposited Surface Area, Particle Number Concentration, Particle Size, and Black Carbon Concentration to Characterize Near-roadway and Biomass Source Emissions. MARILYN WURTH, Brian P. Frank, Gil H. LaDuke, Oliver Rattigan, H. Dirk Felton, Jake Lindberg, Nicole Vitillo, Patricia Fritz, Thomas Wainman, *New York State Dept. of Environmental Conservation*

There is currently an uncertainty about the appropriate metric to use for characterizing ambient ultrafine particles (UFP) and whether such metrics should be source specific. Some researchers have suggested particle surface area – including lung deposited surface area (LDSA) - as a more relevant exposure metric to consider when evaluating health risk because UFP have such a large surface area per unit mass. Studies report a range of particle number concentration (PNC) and LDSA measurements in different environments including urban areas impacted by traffic and residential areas with biomass combustion sources. Differences in source particle size distributions are expected to affect LDSA measurements directly since aerodynamic particle diameter is a key determinant of respiratory tract deposition. More research is needed to investigate how LDSA relates to both particle size and PNC to better understand how UFP and LDSA change spatially and temporally.

This study utilizes portable instruments to obtain simultaneous measurements of multiple characteristics of UFP in different ambient environments to investigate the use of LDSA as an exposure metric. Collocated and simultaneous measurements were conducted for LDSA (Partector, Naneos, Inc.), PNC (CPC 3007, TSI, Inc.), geometric mean particle diameter (NanoScan, TSI, Inc), and black carbon concentration (microAeth MA300, Aeth Labs). Measurements were conducted in three ambient urban environments impacted by traffic emissions: proximate roadway (<5m to roadway), near roadway (<100 m to roadway), and urban background. The LDSA/PNC ratio was evaluated as a potential exposure metric that conceptually represents the percentage of an exposure to a given particle number concentration that is deposited in the lungs; it is also loosely correlated to particle diameter. The results show that both LDSA/PNC and particle diameter in these environments have a nonlinear relationship with PNC. These relationships can be further divided into 3 distinct regimes which are a function of particle diameter, each with a different correlation to PNC. These results have implications both for understanding the differences and similarities of UFP behavior in proximate and near-roadway environments, and in evaluating their potential health impacts. A similar evaluation is performed using a parallel set of simultaneous source measurements from a biomass combustion source in order to investigate the impact of source aerosol on these characterization measurements. A combined metric assessment may help define source profiles and their relative contributions, explain relationships between measurements, and identify which metrics are most useful to evaluate air quality.

7CD.18

Oxidative Potential and Cellular Oxidant Production from Biomass Burning Aerosol. Wing-Yin Tuet, Nilmara de Oliveira Alves, Shierly Fok, Dong Gao, Paulo Artaxo, Perola Vasconcellos, Julie Champion, Rodney J. Weber, NGA LEE NG, *Georgia Institute of Technology*

Biomass burning emissions in the Amazon region drastically change the composition of the atmosphere and may have negative effects on human health. Exposure to inhalable particulate matter (PM) has been associated with increased cardiopulmonary health risks. Results from toxicology studies suggest that PM-induced oxidant production, including reactive oxygen and nitrogen species (ROS/RNS), may be a possible mechanism by which PM exposure results in adverse health outcomes.

Here, we present chemical oxidative potential and cellular oxidant measurements from biomass burning PM samples collected in the southwestern part of the Brazilian Amazon region during the dry and wet seasons (n = 41). The dithiothreitol (DTT) assay was utilized to measure the concentration of redox-active species present in each sample. Murine alveolar macrophages were also exposed to PM extracts for 24 hrs and the resulting ROS/RNS produced as a result of exposure was measured. For all samples regardless of season, a significant positive correlation was observed between ROS/RNS levels and monosaccharide anhydride concentrations, such as levoglucosan. While levoglucosan itself was found to be non-toxic, these results suggest it may serve as an indicator of biomass burning aerosol health effects. Correlations between ROS/RNS production and the concentrations of various polycyclic aromatic hydrocarbons (PAHs), as well as their oxygenated and nitrogenated derivatives, were also examined. Taken together, these results suggest the possible role of PM-induced oxidative/nitrosative stress, which may affect human health.

7CD.19

ROS-Generating Capacity of Particulate Matter over two Cities in Eastern Mediterranean. DESPINA PARASKEVOPOULOU, Irini Tsiodra, Aikaterini Bougiatioti, Athanasios Nenes, Nikolaos Mihalopoulos, *National Observatory of Athens*

The capacity of particulate matter to generate reactive oxygen species (ROS) has been reported as a more important factor of health impairment than the concentration of particulate matter (PM). Although PM-induced oxidative stress has been characterized as a primary mechanism in the initiation of human cell damage, there is no well-established association between composition, sources and the exact mechanism of aerosol oxidative potential (OP) worldwide. Especially in Europe, there are limited studies that involve a relatively short number of data sets. The aforementioned necessity to correlate PM toxicity with aerosol composition and emission sources has led us to the conduction of the present study, in order to assess the adverse health impacts. Two different types of sites were used so that the obtained results are investigated on both temporal and spatial basis. Furthermore, correlations between OP and other aerosol chemical components took place using various measuring techniques, to identify the sources of aerosol OP in each studied site.

Aerosol sampling was conducted, from July 2017 to January 2018, simultaneously at an urban site in the city of Athens (Continental Greece) and at a suburban background site in the city of Heraklion (Island part of Southern Greece). A dichotomous aerosol sampler ($PM_{2.5}$) was used in Athens, while in Heraklion total suspended particulate (TSP) matter was collected through a high volume air sampler. For the determination of PM oxidative potential the acellular method of dithiothreitol (DTT) assay was applied, using an innovative semi-automated system, for conducting the measurement on numerous samples, overcoming the obstacle of time consuming and intense laboring analytical processes. Concurrent estimation of inorganic and organic aerosol components' concentrations was accomplished through Ion chromatography, Aerosol Chemical Speciation Monitor (ACSM), Aethalometer and OC/EC analyzer.

The OP presented higher values in the urban site, where the DTT activity of fine particulate matter gave an average of 0.23 ± 0.11 nmol min^{-1} m^{-3} and seems to be 10 times higher than that of the suburban background site, where the average value of DTT activity for TSP was 0.021 ± 0.013 nmol min^{-1} m^{-3}. The measured OP at the urban and suburban background site ranged between 0.40 ± 0.02 nmol min^{-1} m^{-3} and 0.064 ± 0.005 nmol min^{-1} m^{-3}, respectively, presenting higher values mostly during the days that there was intense biomass burning. These differences in the OP between the two sites were expected since the urban site is located in a densely populated city, where both regional and intense local aerosol sources play an important role in the composition of particulate matter. Furthermore, the investigation of correlation between OP and other PM chemical species indicated that both primary (biomass burning, fossil fuel) and secondary (aged oxidized species, photochemical reactions) aerosol sources can affect to a different extent the capacity of particulate matter to generate ROS, depending on the season of the year and the location of the site.

7CD.20

Surface Area Is the Biologically Most Relevant Dose Metric for Particle-Induced Inflammation in the Lung. OTMAR SCHMID, Kristina B. Knudsen, Sarah Søs Poulsen, Yaobo Ding, Rambabu Atluri, Kirsten Kling, Anne T Saber, Nicklas R. Jacobsen, Keld A. Jensen, Håkan Wallin, Tobias Stoeger, Ulla Vogel, *Helmholtz Zentrum Munchen, Comprehensive Pneumology Center*

As part of the SmartNanoTox project (Horizon 2020, EU-funded) a large body of data on short-term (1d) and intermediate-term (28d) pulmonary inflammation was assessed in rodents after pulmonary application of low-solubility particles. Due to the complexity of inhalation studies with animals there is a much larger body of data on particle induced toxicity employing the technically much simpler route of intratracheal instillation (IT), where of a small volume of a particle suspension is injected directly via the trachea into the lungs. Here rodent studies (mice, rats) were included which determined the pulmonary inflammatory response via neutrophil influx into the lungs and applied at least three different particle doses with a single IT application.

Hundreds of data points published in more than 20 studies from numerous laboratories were included in this overview study comprising ca. 50 different types of (nano-)particles varying with respect to material (six types of soot, graphene, polystyrene, various metal oxides), crystallinity (crystalline, amorphous), shape (spherical, fiber-/tube-like), size (diameter: 9 – 1500 nm, fiber-like: diameter x length 10 – 60 nm x 0.7 – 10 µm) and mass-specific BET surface area (5 – 1000 m^2/g).

After scaling to lung-delivered dose (applied dose per mass of the lung) there was excellent agreement between data from different animal models (mice and rats) and from different laboratories. This lends credibility to conclusions drawn from the combined data sets. Surface area, measured according to the BET method, was identified as the biologically most relevant dose metric explaining about 80% of the observed variability in acute (1d) pulmonary inflammation (R^2~0.8). For comparison, mass and close-packed volume (R^2~0.5), joint length (R^2~0.4), and number of primary particles (R^2~0.2) had a much lower predictive power for particle-induced inflammation.

Moreover, surface area was the only dose metric which allowed clustering of all of these ca. 50 different materials into different classes of toxicity independent of their primary and agglomerate size. At 1d, materials without intrinsic toxicity having EC_{50} values of ca. 175 cm^2/g lung (dose at which 50% of the maximum possible neutrophil influx was observed) could be clearly distinguished from materials with moderate to high intrinsic toxicity such as some transition metal oxides (here: Co, Ni, Zn, Fe; EC_{50}=15 cm^2/g lung) and crystalline quartz (EC_{50} < 5 cm^2/g lung)). It is interesting to note that all types of soot particles, which were investigated here, belonged to the low toxicity class in spite of their very different organic loadings. Moreover, a large number of multi-walled carbon nanotubes (MWCNTs) belonged to the low-toxicity class, but some types of MWCNTs showed enhanced inflammatory response. Prolonged inflammation (here up to 28d) also scaled best with surface area as dose metric and the degree of prolonged inflammation was well predicted by the acute response profile (1d).

This analysis suggests that mainly surface-related modes of action are driving particle-induced pulmonary inflammation. Moreover, lung-deposited surface area (in addition to mass and possibly number) should be measured for the assessment of aerosol-related health effects.

7CD.21

Biofuels: Largest Global Lung-cancer Risk in the 21st Century. SIJIA LOU, ManishKumar Shrivastava, Alla Zelenyuk, Richard Easter, Philip Rasch, Jerome Fast, Staci L. Simonich, Huizhong Shen, Brian Thrall, Shu Tao, *Pacific Northwest National Laboratory*

Polycyclic aromatic hydrocarbons (PAHs), emitted from combustion of biofuels and fossil fuels, are toxic compounds and known to cause lung-cancer. In the future, PAH emissions could vary significantly with regulatory policy and newer emissions control technologies. Thus, it is important to understand how exposure to PAHs and its associated lung-cancer risk could change in the future. In this work, we investigate how lung-cancer risk due to PAH exposure changes under various future emissions scenarios projected by Representative Concentration Pathways (RCPs). Benzo(a)pyrene (BaP) is one of the most carcinogenic PAHs and is used as an indicator of cancer risk from PAH mixtures. All RCPs reduce traditional fossil fuels use and increase renewable and nuclear use in 2050 compared to present-day. Furthermore, most RCPs project increasing cropland use because of the increased food demand with growth in population. Importantly, bio-energy use could increase significantly in the future, which would increase PAH emissions and their associated health risks. Indeed, our simulations indicate that biofuel use will be the largest global contributor to incremental lifetime lung cancer risk (ILCR) in the 21st century. Most of the projected increase in lung-cancer risk due to increased biofuel use is projected to occur in developing countries like those in Africa and South Asia. Developing countries will most likely drive global impacts of PAHs on lung-cancer risks. Advanced residential combustion units that promote complete combustion (such as improved woodstoves) will be essential to reduce PAH emissions and their global health risks.

7CM.2

Effect of Dust Loading on Cleaning of Solar Panels by Electrodynamics. JOSHUA UDVARDY, Jennifer Chesnnutt, Bing Guo, Chang Yu Wu, *University of Florida*

As dust collects on the surface of solar panels, the amount of irradiance reaching the solar cells decreases, which decreases the electricity output of the solar panel. A proposed efficient and cost-effective solution is an electrodynamic dust shield (EDS) that transports dust off the panel by electrodynamic waves. The purpose of this study was to determine the effect of dust loading on the dust removal efficiency of an EDS. An in-house computer code (discrete element method) was used to simulate the transport, collision, and adhesion of charged dust particles subject to two-phase waves on a tilted EDS. Dust removal efficiency was defined as the percentage of dust removed in terms of mass and number of particles. Three different mass loadings of dust particles were simulated, which represented the amounts of dust accumulated on the panel during 1, 4, and 16 days without cleaning, based on 1-day dust accumulation in summer months in Doha, Qatar. Mass and particle removal by percentage was lowest for all simulations for the 1-day dust accumulation case (minimum 11% lower). Mass removal by percentage was considerably similar between cases with 4- and 16-day particle accumulation (minimum 2.3% difference). Although mass removal between these two different loadings was similar by percentage, the mass of particles remaining on the solar panel with the 16-day accumulation case (minimum 723 mg/m2) was larger than that of the 4-day accumulation case (minimum 563 mg/m2), leaving more particles that would result in a lower amount of irradiance reaching the solar cells. Further investigation in the future could analyze the efficiency of particle removal in terms of percent area of the solar panel covered by dust particles after EDS operation.

7CM.4

Collection Performance of Nanofiber/Microfiber Mixed Air Filter Prepared by Wet Paper Processing. Youichi Omori, TIANYI GU, Li Bao, Yoshio Otani, Takafumi Seto, *Kanazawa University*

Recent progress in manufacturing nanometer-order fibers (nanofibers) may lead potential applications of nanofibers to air filtration media. Since nanofibers are expected to enhance the collection performance (a high efficiency at a low pressure drop), the application of nanofiber to air filter has been investigated by several research groups. The quality factor, Q_f, of an air filter is a widely used index to evaluate the filter performance. From our preliminary experiment, Q_f of a commercial air filter (uncharged, medium performance and HEPA grade, fiber diameter of submicron) was around 0.03 Pa^{-1} or less for particles of 300 nm at the filtration velocity of 5.3 cm/s. Based on the filtration theory, mixing of small amount of nanofiber is expected to increase Q_f. However, the structure of nanofiber filter prepared in the most of literatures was thin film (membrane) due to the low mechanical strength of nanofibers and a high packing density. As a result, the filtration performance and the service life of nanofiber filters are not yet high enough to meet the high demand for industrial usage.

In this work, a wet paper processing method was used to produce nanofiber/microfiber mixed filter media. Two kinds of nanofibers (α and β) with the average fiber diameter of 177 and 240 nm were mixed at 10 to 20 wt% with microfibers of the average diameter of 11.6 micron. The filtration experiments were conducted using polyalphaolefin (PAO), NaCl and Japanese standard dust (JIS-11) test aerosol at the filtration velocity of 5.3 cm/s. Three kinds of test filters were prepared with the collection efficiencies of (a) 80%, (b) 99.7%, and (c) 99.99% for 0.3-micron particles by changing the mixing ratio of nanofibers. The pressure drops of these filters (5.3 cm/s) were (a) 42 Pa, (b) 133 Pa and (c) 218 Pa, attaining the quality factor of 0.04, 0.044 and 0.04, respectively. The quality factor is also evaluated based on the single fiber filtration theory (Kirsch and Stechkina, 1978) taking into account the inhomogeneity of filter packing. A good agreement was found between the experimental and theoretical collection efficiencies, suggesting that the wet processing is an effective means for packing nanofibers uniformly in a micron fiber bed.

7CM.5

Development and Performance Evaluation of Venturi Scrubber for Dust & Gases at Vertical Shaft Limekiln Industry.

PRASHIK MANWATKAR, Padma Rao, Anirban Middey, Ashish Patil, *CSIR-NEERI*

In India, small and medium scale industry has also ruined the environment in large scale where the air pollution control system not installed. Limekiln industry with a production capacity of 40 TPD has found a high range of dust and gas, emitted due to calcination process. The average dust concentration in the form of total suspended particulate matter (TSPM) is found to be high in the stack as 364-2033 mg/Nm3, and fourteen various organic gases with different concentration were found at the outlet of the stack. Portable gas analyser Fourier Transform Infrared Spectroscopy (FTIR) and portable dust monitoring kit used for dust (TSPM), and gases are monitoring both an inlet and outlet of the system. To reduce this highly concentrated dust and gaseous pollutants a wet scrubber (venturi scrubber) installed, all gases and dust treated in the venturi scrubber by water and Lime-water, and additional cyclone separator was used to separate gases from a liquid.

The gases and dust are sucked by the blower and then passed through the venturi scrubber where the water sprayed over the pollutants. The gases are then removed from the top of cyclone separator which is then released into the atmosphere through the induced draft fan, and treated liquid is collected in the recirculating tank for recycling. The gas flow rate passing through the venturi scrubber is 8732.34 m3/hr, and the liquid to gas (L/G) ratio is 0.74 L/m3. The gas velocity is 77.25 m/s at the throat corresponding to the gas flow rate of 8732.34 L/min, respectively. For the effective treatment by venturi scrubber, the ratio of L/G should between 0.4-0.9 (Hesketh and Mohan, 2012). Dust controlled with 89.5-99.1%, and 65%-100% reduction in gases was observed.

7CM.6

Control of Particles in the Pulsed Plasma Reactor for SOx Removal. CHANG GYU WOO, Hak-Joon Kim, Yong-Jin Kim, Bangwoo Han, *Korea Institute of Machinery and Materials*

In Korea, 343,161 tons of SOx were emitted in 2014. SOx itself cause various health effects. Besides, fine particles are generated from such gas precursors. For SOx removal, a lot of methods such as scrubber technology and etc. were used. Pulsed plasma is one of the above methods by converting SO_2 gas to $(NH_4)_2SO_4$ particles using pulsed plasma and NH_3 gas. Converted particles can be removed by water-flowing film inside the reactor. SO_2 was controlled by voltage of the pulse power, NH_3 concentration. The gas concentration was measured NDIR measurement equipment and FTIR equipment. Air was supplied to the reaction chamber with 30 m^3/h. Pulsed plasma reaction generated 30~100 nm particles. Gas concentration after this reaction was decreased to lower than 2 ppm. This research can be applied to the reduction facility of SOx emitting factories. This research was supported by the Eco-Innovation Project operated by the Korea Ministry of the Environment.

7CM.7

Numerical Investigations on the Effectiveness of Urban-scale SALSCS under Idealized Atmospheric Conditions by Using a Large-eddy Simulation Model. QINGFENG CAO, Lian Shen, Sheng-Chieh Chen, David Y. H. Pui, *University of Minnesota*

In recent years, many urban regions have been experiencing severe air pollution, adversely affecting the health and living quality of city populations. A Solar-Assisted Large-Scale Cleaning System (SALSCS) was proposed as an innovative strategy aiming at utilizing buoyancy principle to generate airflow in large quantities with solar heating and facilitate the separation of fine particulate matter (PM) from atmospheric air for urban air pollution remediation. Previously, atmospheric simulations have been conducted over the terrain of Beijing in China by using the Weather Research and Forecasting (WRF) model, demonstrating that eight full-scale SALSCSs installed in the suburb of the city can reduce about 11 – 15% of the air pollution concentration in Beijing. In order to further improve the pollution cleaning efficiency of the system, an urban-scale SALSCS has been proposed recently, which has a solar collector and tower with dimensions of less than 120 m by definition, so that it can be directly installed inside city blocks to remove air pollutants and deliver clean air. In the current study, we performed atmospheric simulations by using a large-eddy simulation (LES) model, where large scale motions of a turbulent flow are computed directly and only small scale (sub-grid scale) motions are modelled. To evaluate the effectiveness of urban-scale SALSCS on combating air pollution, various idealized ambient conditions were considered, such as SALSCS operating in quiescent atmosphere or under different ambient wind speeds. Air pollutants and SALSCS airflow pattern have been implemented into the numerical model. The efficiency of urban-scale SALSCS in reducing air pollution concentration within a certain ambient range has been determined quantitatively based on the obtained numerical results. Flow patterns at the SALSCS surrounding regions were studied in detail, and interesting animations were created accordingly.

7CM.8

Mist Removal Performance of a Novel Electrostatic Mist Eliminator Combined with a Flue Gas Desulfurization Process in a Coal-fired Power Plant. Hak-Joon Kim, Kim Jin-Seon, Kim Myungjoon, Bangwoo Han, Chang Gyu Woo, YONG-JIN KIM, Lee Sangrin, *Korea Institute of Machinery and Materials*

As coal-fired power plants have become the main source of particulate matter in Korea recently, the need for improvement in environmental equipment is increasing. Particularly, the Korean government tried to reduce the emissions of fine dust by temporarily shutting down 8 coal-fired power plants from over 30 years old in June 2017. However, coal-fired power plants account for about 40 % of Korea's total electricity production, making it difficult to shut them down or dispose of them immediately. Therefore, in this study, we intend to develop particle removal technology for coal-fired power plants. In general, the flue gas processing systems of the coal-fired power plant are composed of a selective catalytic reduction (SCR), an electrostatic precipitator (ESP), and a wet flue gas desulfurization (FGD). A mist eliminator (ME), a chevron type demister, is installed at the downstream of the FGD, removes particles and mists generated in the FGD. However, the existing ME has low particle removal efficiency because of its principle of particle removal of the inertial impaction. Consequently, in this study, a new type of an electrostatic mist eliminator (EME) was developed and evaluated as an alternative to the ME. Because the space at the downstream of FGD is limited, the EME was designed for a single-stage electrostatic precipitator with parallel charging and collecting plates whose geometry is usually used for two stage ESPs for indoor air quality. High voltage metallic and grounded plates were placed alternately. A lab scale prototype of the EME and ME were investigated to compare particle collection efficiency and pressure drop of the systems. Limestone (CaCO3) aqueous solution used in a FGD was aerosolized by using a twin-fluid nozzle to generate particles, and negative voltage of 10 to 14 kV was applied to high voltage plate of the EME. An optical particle counter and isokinetic particle sampler based on EPA Method 5 were used to measure the changes in particle mass concentrations at the upstream and downstream of the ME and EME. Each experiment was repeated two to three times. When the face velocity of the systems increased from 2 to 5 m/s, the efficiency of the ME against TSP (Total suspended particle) and PM 2.5 increased from 20.0 to 33.9%, and 9.0 to 20.2%, respectively, while the efficiency of the novel EME against TSP and PM 2.5 decreased from 89.1 to 65.0% and 82.3 to 55.6%, respectively, when -14 kV was applied. On the other hands, pressure drop of the ME and EME was varied from 44 to 241 Pa, and 5 to 29 Pa, respectively. TSP removal efficiency measured based on EPA Method 5 was 83.1 and 19.4% for the EME and ME, respectively, when face velocity was 4 m/s. These results indicated that the novel EME has high particle collection efficiency up to approximate 90% compared to the general ME and extremely low pressure drop by approximate 1/10. Therefore, we expect the EME can contribute to reduce the emissions of fine particles from coal-fired power plants.

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7CM.9

Filtration Performance and Particle Loading Characteristics of Various Beaded Nanofiber Filter Media. SEONG KIM, H. Young Chung, David Y. H. Pui, *University of Minnesota*

Nanofiber filter media has been known as promising filtration technology with higher filtration efficiency and figure of merit than conventional filter media. However, relatively high pressure drop due to its high packing density is one of the main drawbacks of nanofiber filter media. In order to overcome this drawback, beaded nanofiber has been introduced to reduce filter pressure drop by providing fiber-to-fiber spaces, that is, intentionally fabricated polymer beads along nanofibers can play an important role to maintain air path through the filter media. Some previous investigations have compared filtration efficiencies and initial pressure drops between conventional nanofiber media and beaded nanofiber media and showed beaded nanofiber media has a higher figure of merit than conventional nanofiber media by reducing the pressure drop through the filters. However, there has not been a systematic study on bead effect on filtration performance and no particle loading study has been conducted yet. In this study, we fabricated various shapes of beads with a controlled concentration on nanofiber media and investigate its effect on filtration performance and particle loading characteristics.

7CM.10

Electrostatic Precipitation of Ultrafine Particles in the Corrosive Gas Condition with a Novel Ion Injection Type Charger. Hak-Joon Kim, YONG-JIN KIM, Bangwoo Han, Chang Gyu Woo, Jong-Pil Yoon, *Korea Institute of Machinery and Materials*

A novel ESP for IT manufacturing industries was developed that uses a ion injection type carbon brush charger to achieve perfect separation from contact of polluted gases, and to impose additional electric field to enhance collisions between ions and particles. The performance of the ESP was evaluated experimentally for particles with a mean diameter of 100 nm based on number, and of 200 nm based on surface area by varying the voltages for chargers and for additional electric field imposing, and number of the chargers. Finally, the collection efficiencies of the ESP were compared with those obtained from the Deutch's collection theory using experimental particle average charges. The total air flow rate for the test were approximate 110 L/min with 10 : 1 ratio of main and mixing flows in the ESP, and applied voltages for chargers and additional electric field were from -10 to -22 kV, and from -5 to -10 kV, respectively. Collection efficiencies in the ESP were linearly proportional to increase in number of chargers and applied voltage to chargers, while those were inversely proportional to increase in applied voltage for additional electric field. The collection efficiency of the ESP for 110 L/min corresponding to flow speeds of 0.19 m/s through the charging stage and 0.23 m/s through the collection cell was reached to over 90% based on total particle number at the applied voltage to triple chargers of -15 kV and additional electric field between upper and bottom plates in charging stage of -6 kV/ 100 mm.

7ES.2

Air Pollution and Control: Past, Present and Future. SHUNXIANG HUANG, *Institute of Chemical Defense*

The essence of air pollution is the impact of air pollutants on human health and environment. The article divides air pollution and control into physical process, chemical processes, and biological, as well as how to describe the three progresses by mathematical methods and to calculate them by computer and reviews systematically their development and interrelationships. This paper summarized the theories, techniques and methods of history, present and existing problems on atmospheric physics, atmospheric chemistry, emission inventory, atmospheric environment monitoring, meteorological field forecast, air quality forecast, source apportionment and tracing source, the impact of air pollution on human health, and atmospheric pollution control. Put forward the theoretical framework, as well as core scientific problems of air pollution hazard identification and control, and pointed out that the theories, techniques, methods and standards of inversion and generation of emission sources, particle toxicity identification, chemical process assimilation, health risk prediction and early warning, synchronization source apportionment of predicting results, and dynamic optimal control are not yet mature, which are the main directions for future development, due to the extremely complicated and staggered influence as well as constraints on physical process, chemical process, biological process as well as mathematical description and computer calculation principle of air pollution and prevention. If the toxicity of pollutants is directly related to health risks, which may provide more direct and effective scientific and technological support for air pollution emergency optimal control as well as the optimal issues of industrial structure adjustment, energy structure adjustment and heavy pollution sources layout, it will play a fundamental role to meet the objective needs of identifying accurately pollution sources, achieving targeted management and promoting ecological civilization construction.

Key Word: air pollution, toxicity identification, air pollution prevention, environment and health

7ES.3

Scattering and Absorption Properties of Aerosols in Amazonia Using Remote Sensing (AERONET) and in situ Measurements. FERNANDO MORAIS, Eduardo Landulfo, Paulo Artaxo, *University of Sao Paulo*

Optical properties of aerosols in Amazonia have been measured over the last 18 years at 8 AERONET sites using CIMEL sunphotometers. Ground based measurements of scattering using TSI and Ecotech three wavelength nephelometers were performed in several sites in Central and Southeast Amazonia. Absorption was measured with Multi-angle Absorption Photometers (MAAP) model 5012 from Thermo Enviroment and AE33 Aethalometers from Magee Scientific. Black carbon was also measured in Nuclepore filters collected in Stacked Filter Units. Measurements were done in Central Amazonia (Manaus ZF2, Manaus EMBRAPA and ATTO tower), as well as in Rio Branco, Porto Velho, Ji Paraná, Santarem and Alta Floresta.

Results shows important geographical and seasonal variability, with 5 main aerosol components: natural biogenic primary aerosol particles, biogenic secondary organic aerosols, biomass burning, long range transported from Africa and urban component. Scattering and absorption Angstrom coefficients helps in separating these different components. Dry and wet season shows very different aerosol characteristics. Very low AOD (ATTO Average = 0.08 ± 0.04) at 500 nm is observed in the wet season, while AOD (ATTO Average = 0.20 ± 0.12, but can reach AOD 3-4 at Alta Floresta and Ji-Paraná) at 500 nm observed in the dry season in Southwestern Amazonia.

7ES.6

Aerosol Size Distributions over the Indo-Gangetic Plains Just Prior to the Onset of SW-Monsoon. MUKUNDA M GOGOI, Suresh Babu, S.K. Satheesh, Krishna K Moorthy, *Vikram Sarabhai Space Centre*

As part of the South West Asian Aerosol Monsoon Interaction (SWAAMI) experiment, we have investigated the three dimensional (spatio-temporal and vertical) properties of aerosol size distribution over three distinct geographic regions of northern India just prior (01 - 20, Jun 2016) to the onset of south west (SW) monsoon. This is based on observations on-board a beechcraft-200 aircraft over Jodhpur (JDR) in the northwestern India, Varanasi (VNS) in the central part of Indo-Gangetic Plains (IGP) and Bhubaneswar (BBR) in the eastern peninsula. Aerosol number size distributions, in general, followed bimodal structures having a prominent mode in sub-micron range (< 1µm), having highest magnitude over JDR, followed by VNS and BBR. Interestingly, aerosol mass size distributions showed higher values (beyond 10µm particle size range) at BBR, while the dominance of fine mode was significant over JDR. Vertically, aerosol total number concentrations (NT) decreased with altitude in the entire size spectra. The variation in aerosol size distributions from surface to the ceiling altitude of aircraft measurement was more conspicuous at VNS. Near the surface, coarse mode aerosol concentrations (NC) decreased from west (JDR) to east (BBR), while the accumulation mode concentrations (NA) remained highest at VNS. Regionally, the day to day variations (corresponding to each distinct flight direction) of the altitudinal distributions of aerosols were more conspicuous at BBR, indicating the contrasting influence of marine and anthropogenic components over near coastal location in the Indian peninsula. Vertical profiles of Black Carbon (BC) mass fractions are also examined for individual days during which the flight sorties were made along distinct directions. BC mass fraction remains lowest at JDR. At VNS, very high values are seen up to 1.5 km (probably the inversion height) above which the fraction steeply falls off. On the other hand, at BBR, though the surface BC fractions were low, it increased steadily with altitude up to 2 km and remained nearly steady thereafter. At BBR, the higher values are BC mass fractions were noticeable when the flight sorties were made over the region of thermal power plants located south west of the BBR base station. Over the same region, concentrations of NO2 and SO2 were also found high, indicating the emissions from coal burning in the region. Aerosol depolarization ratio and aerosol types derived from the cloud aerosol transportation system (CATS) onboard International Space Station (ISS) indicated the presence of dust loading at JDR, mixed with soot in the central IGP and a mixture soot, dust and sea-salt at BBR. Vertical cross section of the values of attenuated backscatter coefficients (from CATS) indicated that the vertical extension of aerosols reached as high as 5 km during the period of observation. Analysis of CloudSat data revealed the stronger influence of aerosols on cloud droplets properties over BBR, where the cloud effective radii were found to be lower in comparison to the values at VNS.

7ES.9

Mineralogically-Speciated and Size-Resolved Global Combustion-Iron Emission Inventory. SAGAR RATHOD, Tami Bond, *University of Illinois at Urbana Champaign*

Global anthropogenic contribution of bioavailable iron to oceans is perturbing the ocean-atmosphere iron and carbon dioxide budget by enhancing phytoplankton growth (primary oceanic productivity) and carbon dioxide uptake. Quantification of iron, its speciation, and its representation in climate models is poorly understood due to the lack of size-resolved observations and mineral-speciation of iron at source and at oceans. This work presents a global size-resolved total and soluble iron emission inventory based on anthropogenic combustion activities. Iron fractions in particulate matter emitted from fuel-technology combinations were compiled and overlaid on a particulate matter emission inventory generated in SPEW (Speciated Particulate Emissions Wizard). The anthropogenic contribution of total iron for the year 2000 was 0.16(0.037-0.56) Tg/yr as PM_1 and 0.20(0.040-1.5) Tg/yr as PM_{10}.

The representation of iron in climate models for their transport and atmospheric processing requires speciated-iron emissions at source. Currently, combustion iron is modeled as a single mineral in the fine mode in CESM. Atmospheric processing is the low-pH iron mobilization in the minerals in particulate matter which enhances its solubility. This work presents speciated-iron emissions at source from combustion activities. Major iron-minerals were grouped into six classes: clays, oxyhydrides, sulfates, sulfides, carbonates, and metals and a temperature-dependent phase transformation model was applied on the initial iron speciation to estimate the iron speciation at different temperatures. Iron in the emission was grouped into clays, oxyhydrides, hematite, magnetite, sulfates, and carbonates which were then coupled with the total iron emissions and mineral-specific solubility. The results from this study will enable models represent and process combustion iron as a combination of different minerals and apply mineral-specific processing scheme.

7ES.10

Evaluation of Six Years of Aerosol Chemical Speciation Monitor Data from the ARM Southern Great Plains Site.

THOMAS WATSON, *Brookhaven National Laboratory*

The first DOE ARM Aerosol Chemical Speciation Monitor (ACSM) users meeting was held on April 11-13, 2017 at Aerodyne Research, Inc., to discuss the Southern Great Plains (SGP) ACSM data quality and establish best practices for data collection and processing. The participants examined six years of calibration and processed data. Specific issues raised by data users were addressed and case studies from two field experiments and the most recent data from the ACSM installed in the newly commissioned SGP Aerosol Mobile Facility 7 (AMF7) were examined. The participants recommended that the SGP ACSM data be reprocessed using calibration values averaged over the history of SGP ACSM calibrations. They also recommended that the data quality be evaluated by comparing (1) observed versus predicted particulate ammonium (NH4+) mass loadings, and (2) ACSM mass loadings versus mass loadings calculated from particle size and light scattering data. The contents of the data streams from the ACSM were defined based on ARM requirements and the necessary tasks to implement these recommendations were assigned to the mentor and the instrument manufacturer.

Six years of data are evaluated using the criteria developed at the users' meeting, with particular attention to the comparison of ACSM total mass loading to mass loadings calculated from SMPS, and UHSAS particle size distribution data.

7ES.11

Aerosol-Induced Changes to Cloud Radiative Forcing over Indian Subcontinent. ABIN THOMAS, Vijay Kanawade, Chandan Sarangi, S.N. Tripathi, Srilakshmi Sunkara, *University of Hyderabad*

Aerosol-cloud interaction is the most considerable uncertainty in the Earth's radiation budget. The variability of aerosol species and concentration along with the complexity of interaction mechanisms make it hard to quantify the aerosol effect on clouds. The aerosol impact on marine clouds and its changes in the micro- and macro-physical properties are reasonably better understood than its continental counterparts. Here, we investigate the effect of aerosols on the micro- and macro-physical properties of clouds over Indian subcontinent using long-term (2002-2016) satellite (MODIS, CERES, and CLOUDSAT) datasets. We analyzed the aerosol impact on the cloud radiative forcing on instantaneous to seasonal scale.A higher fraction of deep convective and cirrostratus clouds were observed during the monsoon season leading to a higher negative net cloud radiative forcing. The aerosol-induced cloud invigoration is found to enhance the net cooling effect of clouds on the top of atmosphere and surface during Indian summer monsoon season. Overall, the estimated impact of aerosols on the cloud albedo was found to be higher than that on the cloud cover over Indian subcontinent.

7ES.12

Investigation of Concentration Variability, Sources and Atmospheric Transformations of Short-lived Climate Pollutants (SLCPs) at the Rural-site of Indo-Gangetic Plain (IGP), India. Jai Prakash, Harsh Raj Mishra, Atul Kumar, Bhilok Chand, Mattias Hallquist, Gazala Habib, Geetam Tiwari, Jan B. C. Pettersson, Johan Boman, Håkan Pleijel, RAVI KANT PATHAK, *University of Gothenburg, Sweden*

Short-lived climate pollutants (SLCPs) such as light absorbing (at 375 nm) organic aerosol referred as ultra-violet particulate matter (UVPM), black carbon (BC), ozone (O3), carbon monoxide (CO), and nitrogen oxides (NOX) are thought to have significantly contributed to climate change both regionally and globally and adverse human health. However, the quantification of climatic effects of SLCPs such as BC and O3 remain poorly understood. The increasing importance of SLCPs compared to previous studies are attributed to new emission estimates and their sources especially for the people living low-and-middle-income (LMI) rural areas in the Western Pacific and South East Asia including India. Therefore, it is of critical importance to assess the characteristics of SLCPs in India, specifically in the Indo Gangetic Plains, which is a major hub of biomass burning led pollution and atmospheric brown clouds. Further, understanding the aerosol transformation and inter-linked atmospheric processes in the IGP region becomes imperative for developing robust modeling tools to predict their impacts on global climate, human health, and ecosystem. For the first time in India, this study investigated the variability of short-lived climate pollutants (SLCPs) at a long-term measurement rural site in IGP region called "Indo-Gangetic Plains Centre for Air Research and Education (IGP-CARE). The IGP-CARE site is situated in agricultural fields adjacent to a forest by the River Burma (a tributary of the River Betwa) surrounded by six villages in the Hamirpur district, Uttar Pradesh, India. In the present work, the SLCPS (UVPM, BC, O3, CO, and NOX) were continuously measured real time during the period of January 2017 to December 2017 at the IGP-CARE and also recorded parallel meteorological data such as temperature, relative humidity, wind speed, wind direction. During the study period, the annual average UVPM, BC, O3, CO, and NOX were observed 4.0 ± 2.8 μg m−3, 2.8 ± 1.8 μg m−3, 30.4 ± 20.9 ppbv, 497 ± 376 ppbv, and 6.4 ± 2.9 ppbv, respectively. Seasonally, highest concentrations were observed in summer time followed by winter and autumn for O3 and highest concentration was found in winter and autumn for UVPM, BC, CO, and NOX. O3 showed highest diurnal variation (38 ppbv) during daytime and lowest (10 ppbv) during late evening as well as early morning hours. Interestingly, in diurnal pattern of winter season, BC concentration was observed 4.0 μg m−3 almost constant during day and night time, while UVPM showed highest (8.0 μg m−3) during late evening as well as early morning hour. Also for the other seasons, UVPM/BC ratio showed a significant diurnal variability. These indicate that UVPM and BC although co-emitted from the biomass burning, undergo different atmospheric transformation and their ratio is likely to be influenced by temperature or light intensity as the ratio of UVPM/BC was lowest at the noon time. The UVPM represents the fraction of brown carbon (BrC) in aerosol and suggests that light absorbing aerosol compounds are sensitive to either light or temperature or both. Interesting chemistry of UVPM from the biomass burning is yet to be explored. For the source investigation and contribution of local or regional sources and UVPM/BC, O3/BC, O3/CO, BC/CO, UVPM/NOX, O3/CO ratio will be characterized and presented using air mass back-trajectories during the sampling period. Furthermore, the loss of BC and O3 during transport with temperature and RH will be also discussed for the coatings of aged particles by water-soluble compound from this region would be the most likely chemistry of atmospheric processes.

7ES.13

Hygroscopicity and Mixing State of Fine Aerosols in the South Eastern Mediterranean Sea and around the Arabian Peninsula during the AQABA Campaign. SPYRIDON BEZANTAKOS, Konstantinos Barmpounis, Michael Pikridas, George Biskos, *The Cyprus Institute, Nicosia, Cyprus*

Ultrafine aerosol particles in the atmosphere affect the global climate by absorbing and scattering radiation and by acting as Cloud Condensation Nuclei (CCN). Due to the high variability of their physical and chemical properties, however, quantifying their contribution on climate is a challenging task. Particle properties may change depending on the activity of their sources and the meteorological conditions. In addition their mixing state can vary with time and location. Having information about the variation of the properties and the mixing state is therefore very important for understanding the contribution of atmospheric particles on climate.

Here we report the hygroscopicity and mixing state of fine aerosol particles (i.e., particles having dry mobility diameters from 60 to 160 nm), which were measured using a custom made hygroscopic tandem differential mobility analyzer (HTDMA) during the Air Quality and climate change in the Arabian Basin (AQABA) ship based campaign that was conducted from early July to the end of August 2017. The ship crossed the southeastern Mediterranean Sea (SEMED), the Red Sea (RS) and circulated the Arabian peninsula (AP). All these areas pose an increased climate and health related scientific interest as they are affected by multi-source, multi-regional aerosols, which interact, depending on the meteorology patterns. In addition, measurements reporting the physicochemical properties of aerosol, and more specifically its hygroscopicity, are scarce in the middle east, in contrast to the SEMED region. Except from the hygroscopic growth of the sampled aerosols, which is directly derived from the HTDMA measurements we also report their mixing state and their apparent κ-value, connected with different wind patterns, across the path of the ship.
A first analysis of the results shows that the apparent hygroscopic parameter κ of the fine aerosol fraction maxed at approx. 0.4 throughout the campaign, excluding times when the measurements were affected by our ship plumes. Larger (e.g., accumulation mode) particles exhibited values close to this maximum in the proximity of the gulf of Oman, while in the majority being internally mixed, which is indicative of aged/long transported particles, containing a significant amount of sulfates or other highly hygroscopic material. In contrast, the smallest (i.e., 60 nm) aerosols exhibited lower κ values, possibly due to increased soot content, while their highest hygroscopicity was observed in the SEMED region, south of the island of Crete, due to the Etesian outflow. Highest fractions of externally mixed particles in all sampled sizes were observed in the Suez canal due to increased density of local sources (e.g., ship traffic).

7ES.15

Correlations between PM2.5 Concentration and Local Meteorological Conditions with Focus on Statistical Models to Retrieve Long Term PM 2.5 Proxy Data: A Case Study in Chengdu, China. LEI LUO, Xinying Tang, Pengping Wu, Ling Wang, *Institute of Plateau Meteorology, CMA, Chengdu*

The metropolitan city of Chengdu in south-west china has been suffering from severe air pollution for many years due to its basin topography as well as unfavorable atmospheric conditions. During heavy pollution episodes in the city, PM2.5 is mostly the primary pollutants, particularly in winters. With governments implemented stringent emission reduction measures, the local anthropogenic pollutant source usually remains constant or even declined sometimes; therefore meteorological conditions must have been playing a major role in those pollution episodes. To get a clearer understanding on how PM2.5 concentration correlated with meteorological parameters, 3 year's hourly meteorological and PM2.5 data from 2012 to 2014 were obtained from local observation stations. Linear regression and multi-variance analysis were applied to find the correlation between major meteorological variables and PM2.5 concentrations. The preliminary results showed that air temperature, pressure, relative humidity (RH) and wind speed may have caused significant different PM2.5 concentration levels. However, these meteorological factors demonstrate different effects to PM2.5 in different seasons. During the winter, RH has a significant positive correlation while temperature and pressure show a slightly negative correlation with PM2.5 concentrations, but these effects are not obvious in summer. Analysis also reveals that visibility has a strong positive linear correlation with PM2.5, this leads to the idea to derive a statistical model using visibility values to calculate long term proxy PM2.5 data for early history years. This proxy PM2.5 datasets may be very useful in assessing long term aerosol climate effects. Intensive stepwise recursive regression were conducted on dataset of 2013, resulted in a simple yet quite effective statistical model (R=0.67) with visibility variables contributes the most variance. The equation was used on 2012 dataset to calculate proxy PM2.5 concentration for each sample hour in 2012. The retrieved data agreed ideally with the observed PM2.5 concentrations with no significant statistic differences.

7ES.16

Spatial and Temporal Variation Aspects of Aerosol Black Carbon Concentration over India. RAVI RANJAN KUMAR, Vijay Kumar Soni, Sateesh M., M.K. Jain, Sanjay Bist, Siddhartha Singh, *India Meteorological Department*

Black Carbon is one of the very important short term climate forcing agents and a little change in its concentration can considerably affect the climate. Considering its importance India Meteorological Department has established a network of 16 Aethalometers (AE-33) for continuous measurement of equivalent black carbon (EBC) concentration over India. In the present study data have been collected at a time stamp of one minute at Amini, Bhuj, Chandigarh, Guwahati, Jodhpur, Kolkata, New Delhi, Nagpur, Pune, PortBlair, Ranchi, Ranichauri, Srinagar, Thiruvanantpuram, Varanasi and Vishakhapatnam stations for the year 2016. The variation of concentrations was examined with ANOVA (analysis of variance) and F-test. ANOVA and F-tests assess the amount of variability between the group means in the context of the variation within groups to determine whether the mean differences are statistically significant. The calculated F value for daily means is 136 and for 16 stations daily mean data we get a degree of freedom (15,5264). On comparing this F value in the Table at a significance level of 0.05 and (15,5264) degree of freedom, it was found that F values is greater than its critical value so null hypothesis is rejected and hence there is a significant variation in the daily mean data of different stations. F values were also calculated for monthly, seasonal and diurnal variations among all 16 stations and it is 8.6, 5.2 and 47.2 respectively. On comparing these F values according to their degree of freedom (15,168), (15,62), (15,368) respectively at 0.05 significance level, all three exceed its critical values and hence showing significant monthly, seasonal and diurnal variation of EBC concentration. North Indian stations are land locked showing higher concentration of black carbon than coastal stations of south India. Mega cities like New Delhi and Kolkata have very high concentration of EBC and apart from these other stations located in Indo-Gangnetic Plane also show high EBC concentration. The annual mean EBC concentration is depicted on geographical map of India. Most of the north Indian stations show high BC concentration during month of November, December and January and minimum during rainy season. Seasonal variation of EBC concentration is also discussed.

7ES.17

Declining Dust over the Indian Sub-Continent: Signature of a Changing Regional Climate. Velu Vinoj, S.K. PANDEY, Kiranmayi Landu, Suresh Babu, *IIT Bhubaneswar*

Desert dust over the Indian region during pre-monsoon season is known to strengthen monsoon circulation, by modulating rainfall through the elevated heat pump (EHP) mechanism. In this context, an insight into long term trends of dust loading over this region is of significant importance in understanding monsoon variability. In this study, using long term (2000 to 2015) aerosol measurements from multiple satellites, ground stations and model based reanalysis, we show that dust loading in the atmosphere has decreased by 10 to 20% during the pre-monsoon season with respect to start of this century. Our analysis reveals that this decrease is a result of increasing pre-monsoon rainfall that in turn increases (decreases) wet scavenging (dust emissions) and slowing circulation pattern over the Northwestern part of the sub-continent.

7IA.1

Diurnal Variation of Particle Mass Concentration at Underground Subway Tunnel near the Platform. Sang-Hee Woo, Jong Bum Kim, GWI-NAM BAE, Moon Se Hwang, Hwa Hyun Yoon, *Korea Institute of Science and Technology, Seoul, Korea*

Metal particles are known to be generated by train wheels and rail or pantograph and electric wire friction during train operation (Aarnio et al., 2005; Salma et al., 2007). Subway particles are more toxic and higher concentrated than urban street particles (Johansson and Johansson 2003; Kalsson et al. 2005). These metal particles have adverse health effect to passengers and workers (Johansson and Johansson 2003; Aarnio et al., 2005). Therefore, many measurements of particulate matter were made in the subway environment (Johansson and Johansson 2003; Aarnio et al., 2005; Salma et al., 2007; Midander et al., 2012; Zhang et al., 2017). According to worldwide studies, PM10 and PM2.5 in subway platforms and inside train were 41-469 $\mu g/m^3$ and 21-258 $\mu g/m^3$, respectively. Most of them were over WHO 24-hour and annual air quality guideline of 50 and 25 $\mu g/m^3$, respectively. Generally, tunnel has higher concentration than platform, because tunnel was direct sources of particle contamination (Jung et al., 2010). However, characteristic of particle concentration at underground subway tunnel have not been understood well.

In this study, particle concentration was measured in every 2 seconds at subway underground tunnel near the platform. Measurement was made at tunnel adjacent Janhanpyeong station platform, Seoul Metro Line 5, Republic of Korea. Time-series data was analyzed by subway operation. The particle concentration was increased proportionally to the frequency of subway operation. However, it showed a fluctuation due to complex induced airflow by train movement. This pattern of particle mass concentration variation in the tunnel near the platform was different from that in the middle tunnel conducted by authors. Unlike the middle tunnel, opposite side train effect was shown in tunnel near the platform. Similar to the middle tunnel pattern, diurnal variation of particle mass concentration could be predicted by the pattern of particle mass concentration caused by train operation.

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7IA.2

Generation Characteristics of Nanoparticles Emitted under Subway Cabin in Operation. YONGIL LEE, Kyomin Choi, Wonseog Jung, Taesung Kim, Duckshin Park, *Korea Railroad Research Institute*

In this study, measurements were carried out to identify the generation characteristics of wear particles emitted from under a subway cabin during operation. Along with a fast mobility particle sizer, probes were installed under a subway cabin and in a subway tunnel to measure the size distributions of nanoparticles at 1-s intervals. Based on the particle density measured under the cabin minus that measured in the tunnel, the size distribution of wear particles generated under the cabin during deceleration was estimated to be bimodal at 165.5 and 6.98 nm. These particles were most likely generated from wheel–rail contact, as the train utilized electric braking. In addition, a change in the wear mechanism appears to have arisen due to increasing temperature of the wheel–rail contact when nanoparticles were being emitted, leading to initial generation of 165.5 nm particles, followed by 6.98 nm particles 1 s later.

7IA.3

Indoor Black Carbon and Particle Number Concentrations at Two Intercity Bus Terminals in Taipei City. YU-HSIANG CHENG, An-Chi Li, *Ming Chi University of Technology*

Taipei City is the capital of Taiwan as well as an important economic and political center. It is also a main transportation hub in the north Taiwan area. Taipei Bus Station and Taipei City Hall Bus Station are two main transportation hubs providing over 100 intercity bus routes in Taipei City. The design of these two bus terminals are unlike other stations worldwide. These two bus terminals are located inside the modern commercial buildings, housing a shopping mall and several cinemas. Air quality inside these two terminals must be monitored as over 3000 buses are scheduled to run daily in the indoor environments. The particulate matters emitted from buses can accumulate within this semi-confined space, adversely affecting the health of passengers. Therefore, the air quality inside these two bus terminals is an important health concern for passengers, as many passengers spend a considerable amount of time waiting for buses. This study investigated the short-term exposure levels of black carbon (BC) and particle number concentrations for passengers at the ticket booths and waiting areas of these two bus terminals. Four sampling sites, T1–T4, were selected in the Taipei Bus Station, and three sampling sites, C1–C3, were selected in the Taipei City Hall Bus Station. Additionally, the outdoor roadside site about 10 m from the entrance at the bus terminal, TOR and COR, was also sampled. In this study, microAeth AE51 and TSI 3007 CPC were used to measure the indoor BC and particle number concentrations, respectively. A total 40 times of sampling was taken at each selected site between May 2016 and April 2017. Measurement results showed that 15-min BC mass concentrations at Taipei Bus Station and Taipei City Hall Bus Station were 6.3–16.0 and 2.7–7.2 μg m^{-3}, respectively, on average. Additionally, average particle number concentrations at Taipei Bus Station and Taipei City Hall Bus Station were 2.5×10^4–4.2×10^4 and 2.3×10^4–3.4×10^4 particles cm^{-3}, respectively. The highest average BC mass concentration and particle number concentration could be observed at T2 and T4, respectively. The indoor BC and particle number concentrations at the bus terminals were about 1.1–6.1 and 0.7–1.3 times comparing to those at outdoor roadsides, respectively. Moreover, measurement results suggested that the 15-min BC concentrations were positively correlated with particle number concentrations at these sampling sites. Clearly indicating that BC and ultrafine particulate matters can be from the same emission source, which could be buses. Moreover, the concentrations of BC and particle number at these two bus terminals could be affected by their different designs of interior spaces and ventilation systems.

7IA.4

Assessment of Indoor Air Quality in a Beauty Salon. Estela Vicente, Carlos Blanco-Alegre, Fernanda Oduber, Ana Isabel Calvo, Amaya Castro, Roberto Fraile, Mário Cerqueira, Teresa Nunes, CÉLIA ALVES, *University of Aveiro*

The products and treatment techniques used in beauty salons can put both the employees and clients at risk of exposure to high levels of pollutants and hazardous chemicals. A one-week sampling campaign was conducted from 20th to 24th November 2017 in a hairdresser salon in the city of Léon, Spain. The salon is continuously open for 10 h from Monday to Friday. The number of customers was monitored for each sampling day, as well as the treatment of each one. Customers were either habitual or occasional, generally of both sexes, with a higher proportion of men. The space layout includes a reception and waiting area at the front, two hairstyling areas, a waxing room and a dispensary room in the back. Most hair care and hairstyling products are stored in the latter room. The salon offers a wide range of services including manicures, pedicures, waxing services and hair styling/coloring. Temperature, relative humidity, CO_2, CO were continuously monitored with air quality probes inside (TSI, model 7545) and outside (Gray Wolf®, WolfSense IQ-610) the salon. Real-time laser photometric instruments (TSI, DustTrak DRX 8533) were used to record particulate matter concentration profiles over time in the indoor and outdoor environments, simultaneously. All the continuous monitoring instruments were operated with 1-min resolution. Simultaneous sampling with two PM_{10} high volume air MCV (model CAV-A/mb) instruments for gravimetric quantification was carried out. The equipment was operated at a flow of 30 m^3/h. Samples were collected during the opening hours, simultaneously indoors and outdoors. Nighttime samples were also taken in order to compare the PM levels during occupancy and non-occupancy periods. Particulate samples were collected on pre-weighed 150 mm quartz fibre filters (Pallflex®) for gravimetric and chemical analyses. The gravimetric quantification was performed with a microbalance (XPE105 DeltaRange®, Mettler Toledo). After gravimetric determinations, thermo-optical analysis of PM_{10} filters was performed to obtain the carbonaceous content. Samples for formaldehyde and acetaldehyde quantitative analysis were collected on Sep-pak® DNPH-silica cartridges (Waters) connected to a calibrated sampling pump to provide a volumetric airflow rate of 2 L/min. The samples were analyzed via HPLC. Three samples per day, covering the working hours, were collected in three different days of the sampling campaign.

Temperature readings recorded throughout the sampling campaign were not within the ASHRAE (American Society of Heating, Refrigerating, and Air-Conditioning Engineers) comfort zone (winter range), particularly in the morning hours. CO_2, a constituent of exhaled breath that can be used to evaluate if adequate quantities of fresh air are being introduced into a building, showed an increasing level during the day, and decreasing levels during the night. The CO_2 concentrations correlated linearly with the total number of clients attending the salon ($R^2 = 0.721$). There was a strong linear relationship between the photometric and gravimetric PM measurements ($R^2 = 0.927$). From the gravimetric measurements, PM_{10} concentrations of 89 ± 39, 22.8 ± 2.1 and 50 ± 12 $\mu g/m^3$ were recorded indoors during the occupancy and non-occupancy hours, and outdoor air, respectively. Although PM_{10} concentrations were not correlated with the total number of clients, good correlation was found with the number of female customers in the salon ($R^2 = 0.805$). The mean PM_{10} indoor to outdoor ratio was 1.97. Total carbon accounted for 34.1 ± 2.2, 27.3 ± 3.0 and 25.0 ± 5.2 %wt. of the PM_{10} mass indoors during the occupancy and non-occupancy hours, and outdoor air, respectively. The indoor formaldehyde concentration was 11.5 ± 3.5 $\mu g/m^3$, which is below the short-term guideline recommended by WHO to prevent sensory irritation in general population. The acetaldehyde concentration was 9.0 ± 4.7 $\mu g/m^3$.

7IA.5

The Impact of Tobacco Heating System on the IAQ in a Night Club Environment. DAINIUS MARTUZEVICIUS, Marija Meišutovič-Akhtarieva, Tadas Prasauskas, Darius Ciuzas, Karolina Keraitytė, Violeta Kaunelienė, *Kaunas University of Technology, Lithuania*

INTRODUCTION. The adverse effects of traditional cigarette usage to not only the smoker but also to indoor environment have been long established. During recent years, new nicotine containing products increasingly penetrate the market. Such devices are not based on the pyrolysis of tobacco, but on the heating of propylene glycol based liquid containing pure nicotine (such as in electronic cigarettes), or distilling nicotine from specially prepared tobacco in reduced temperatures (such as in tobacco heating systems). These techniques have potentially lower release of secondary pollutants, but the data on their potential impact to IAQ is very rare. This study was aimed to the assessment of the usage of the tobacco heating system to the real-life night club environment.

METHODS. The experimental setup was established in a nightclub, operating at premises of a flow area of approx. 198 m^2, and a volume of approx. 800 m^2. Background aerosol concentration has been measured without any occupancy, followed by the occupancy of 10 and 30 persons. Further tests included 10 and 30 persons using tobacco heating systems (IQOS, Philip Morris Ltd.) simultaneously at a confined space of the club without additional occupancy or activities. The other set of tests were conducted during the full operation of the night club again 10 and 30 persons using the THS. Such design was selected in order to identify if the usage of THS has a significant impact on air quality if used indoors in a rather intense otherwise public environment. The smoking of traditional and electronic cigarettes was prohibited in the nightclub, but some polluted air was leaking into the club from the smoking room located adjacent to the main hall.

ELPI+ (Electrical Low Pressure Impactor, Dekati Ltd., Finland) has been operated at a single location of the night club, drawing samples at a flowrate of 10 lpm at a 1s resolution. Two Tygon sampling tubes have been connected to ELPI+ via a two way switching valve, operating at a 300 s interval. Such designed allowed sampling interchangeably from two locations at a club – one at an area of the usage of THS, another at the opposite side of the club.

RESULTS. During the controlled experiment and without operating ventilation, the background aerosol concentration stayed at a level of 4E+3 - 8E+3 cm^{-3}. The usage of 10 devices simultaneously resulted in 3E+4 - 8E+4, and the 30 instruments resulted in further increase to 1E+5 - 3E+5 cm^{-3}. These increases were reduced back to the background levels after a 30 min of continuous ventilation. The full scale operation of the club has resulted in background values of 5E+4 to 8E+5 cm^{-3}. Such levels are attributed to the mixture of aerosol from kitchen and fugitive emissions from smoking room. No significant effect of the usage of THS devices has been registered in such scenario. This suggests that tobacco heating systems did not produce significant amount of aerosol to influence already high values in the club, but the effects to the bystanders may be still sensible, as confirmed by the increase of concentrations during usage of THS devices with no other activities present.

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7IA.9

A New Computer Model for the Simulation of Secondary Organic Aerosol Formation from Stir-frying Additives Using Aspen Plus. MEHDI AMOUEI TORKMAHALLEH, Fariza Aldemkhan, *Chemical and Aerosol Research Team, Nazarbayev University*

The formation of volatile organic compounds (VOCs) and particulate matter (PM) indoors as a result of cooking are becoming one of the major topics of interest in environmental engineering, due to their increasing hazardous effects on inhabitants. In this study, the simulation of stir-frying corn oil with food additives, namely, myrcia and salt, was developed using Aspen Plus. According to Amouei Torkmahalleh et al [1], this approach presents the results for the time instant at which the operating conditions are established. The scope of this investigation is to determine the chemical composition and physical properties of primary organic aerosol (POA) and secondary organic aerosol (SOA) produced from stir-frying myrcia. Since, the herbs are mainly composed of terpenes [2], it is expected to have significant SOA compounds produced from ozonolysis of terpenes. Furthermore, the effect of cooking temperature on the formation organic PM was investigated. Aspen Plus V9 was employed to simulate the cooking process. In order to estimate the phase equilibrium in vapor and liquid phases a Non-Random Two- Liquid (NRTL) model and Ideal Gas law were applied. Missing parameters were estimated via UNIFAC method, which considers the contribution of present functional groups on the properties of the compound of interest. Indoor VOC and major pollutants including sulfur dioxide, nitrogen dioxide and carbon dioxide were included to air to show their interaction with emissions from cooking. There are three reactors where hydrolysis of oil, oxidation of free fatty acids and ozonolysis of terpenes are simulated. Products of free fatty acids oxidation and terpene ozonolysis were inserted according to existing literature. The outputs from these reactors were mixed with air and cooled to represent rapid dilution and condensation of precursor gases leading to aerosol formation. Finally, Flash block was employed to separate formed aerosol from VOC.

The POA from high temperature frying with myrcia is dominated by terpenes, terpenoids and other aromatic compounds. There are other compounds emitted as well including aldehydes, alkanes and ketones; however they are present in significantly lower amounts. Due to high composition of ring structures, POA possesses relatively high viscosity of 0.0092Pa-sec. Density of the liquid mixture is governed by α-humulene, because it contributes to 93% of the total POA and equals 1.021g/ccm. After introducing excess ozone to cooking emissions, the composition of SOA from stir-frying myrcia was determined. It is governed by products of myrcene oxidation including Hydroxyacetone, 4-vinyl-4-pentanal, 4-oxopentanal and 2-vinyl-pentandial. It is followed by products of α-pinene ozonolysis: acetone, formaldehyde, pinonaldehyde and norpinic acid. Lastly, limonene oxidation yielded 4-acetyl-1-methylcyclohexane, 3-isopropenyl-6-oxo-heptanal, dihydrocarvone and limononic acid. As noted, SOA is comprised of linear structures, therefore its viscosity is significantly lower than that of POA and equals 0.00098Pa-sec. That is, POA was approximately 10 times more viscous than SOA, but the densities of POA and SOA are quite similar, such that density of SOA was estimated to be 1.028 g/ccm. In conclusion, mass percentage of the corresponding products from myrcene, limonene, and a-pinene were estimated to be 68%, 24.34% and 7.66% respectively. Myrcia appeared to increase the rate of particulate matter formation. Heating corn oil to 240 °C produced 10 times less POA than stir-frying myrcia in corn oil. Moreover, stir-frying of myrcia produced nearly 3 times more SOA that heating corn oil alone.

7IA.10

Atmospheric Particulate Matter: A Threat to the Health of Raffaello. PAOLA FERMO, Valeria Comite, Silvana De Iuliis, Carlo Giglioni, Stefania Gilardoni, Davide Gulotta, Francesca Migliorini, Lucia Toniolo, *University of Milan, Italy*

Indoor air quality in historical buildings and museums is receiving increasing concern nowadays among the scientific community. Many sources of pollutants, both gases and particles, are responsible for the accelerated dacay of the works of art. Knowing the levels of indoor pollutants is of critical importance to apply conservation and preservation strategies of cultural heritage.

Air quality at the Ambrosiana Art Gallery in Milan has been monitored (in the period October-November 2017) inside the room where the preparatory cardboard of the School of Athens (1509-1511), one of most important works by Raffaello Sanzio, is stored. This cardboard represents one of the most important works of art present in Milan.

The cardboard is currently undergoing restoration and will be placed in a new case that must be realized taking into account the environmental and microclimatic conditions of the room. The objective of this study was to monitor the concentration and chemical composition of the aerosol particulate matter, up to the nano fraction, which represents the most dangerous for the works surfaces.

The instrumentation used includes:
- a PTS sampler (total suspended powders) (Tecora, Pollution Check, Bravo M2)
- a DustMonit (Contec) analyzer that measures the concentration of dust up to PM1 and provides 13 granulometric classes (up to 300 nm)
- a NanoScan, Nanoparticle sizer 3910 (TSI) instrument that measures particles concentration up to 10 nm
- a SIILIS instrument (Sphere-integrated LII Spectrocopy) that measures, through the laser glow, the particles of black carbon
- a micro aethalometer (AE51 Magee Scientific) for the determination of back carbon.

Some tools have been dedicated to the determination of black carbon which is the main responsible for the blackening of the surfaces.

PM monitoring has been carried out in two museum rooms: the room with the masterpiece form Raffaello and another room visited by a great number of people. The results obtained have shown that outdoor environment can significantly affect indoor air quality. The presence of people can result in increased concentrations of indoor pollutants. From the data acquired by the DustMonit instrument it has been evidenced that PM2.5/PM10 ratio is in most cases very close to 1 indicating a predominance of the fine fraction.

Quartz fiber filters were employed to collect PTS samples. The filters have been fully chemically characterized: main ionic constituents and the carbonaceous fraction (i.e organic carbon, OC and elemental carbon, EC) have been analyzed by IC (ion chromatography) and TOT (thermal optical transmittance) respectively. It is worth noting that the contribution of EC to PTS mass is not negligible. The values obtained are in a fairly good agreement with black carbon (BC) concentrations measured by SIILIS instrument. Furthermore comparing BC values with particles distribution determined by Nano Scan, it is quite evident that BC is mainly present within the fraction with diameter lower than 200 nm which represents a serious threat for the works of art stored in the gallery.

7IA.11

Effect of a Two-Stage Type Electrostatic Precipitator on Collection Efficiency and Ozone Concentration. KOJI YASUMOTO, Hidetoshi Sawano, Kohei Ito, Akinori Zukeran, *Kanagawa Institute of Technology*

Electrostatic Precipitators (ESPs) have been extensively used for the cleaning of industrial process flue gases, combustion flue gases and ventilation flue gases for road tunnels, etc. A home air cleaner is also one application of ESP. However, such air cleaners which utilize corona discharge must be improved the collection efficiency without increasing ozone concentration.

In this study, the collection efficiencies and the ozone concentrations were measured in a single-stage ESP and a two-stage type ESP.

The two-stage type ESP has a discharging section and an electrostatic section. The discharging section (single stage ESP) has a wire-and-plates configuration composed of a high-voltage application wire electrode (f: 0.45 mm, L: 70 mm, SUS304) placed between grounded plate electrodes (70×270 mm) with a gap of 10 mm. The electrostatic section has a parallel-plate electrode structure composed of a high-voltage application electrode (70×174 mm) sandwiched between grounded plate electrodes (70×174 mm) with a gap of 10 mm. All plate electrodes are made of stainless steel with a thickness of 0.8 mm. Room air was used, and the gas flow velocity was adjusted to 0.5 m/s by a fan located on the downstream side of the ESP. Maximum voltages of DC -12 kV and DC -9 kV were applied to the discharging and the electrostatic sections using high voltage generators. 1, and discharge current was measured. Ozone concentration was measured using an ozone monitor at the downstream side of the ESP. The number concentrations for the particle size between 0.3 and 5 mm at upstream and downstream sides of the ESP were measured using particle counters, and the collection efficiency was calculated by equation (1).

$\eta = (1-N_{Dd}/N_{Ud}) \times 100\ \%$ (1)

As a result, the collection efficiency increased as the particle diameter increased due to increasing the charge in the single stage ESP. The efficiency improved with increasing applied voltage, however ozone concentration also increased. This cause is that the reaction between O2 and O generated by dissociation increases with increasing discharge current.

In the two-stage type ESP, the applied voltage on the discharging section was 9.37 kV at any voltage applied to the electrostatic section. The collection efficiency improved with increasing applied voltage to the electrostatic section with increasing the migration velocities of charged particles in the electrostatic section. The discharge current was constant in the discharging section, whereby the ozone concentration at any voltage was approximately 1 ppm. Furthermore, the energy consumption did not increase, since current did not flow in the electrostatic section. Therefore, it was clear that the collection efficiency could be improved without increasing ozone concentration and energy consumption in the two-stage-type ESP.

7IB.1

Potential for Long-Distance Atmospheric Transmission of Influenza Virus. LINSEY MARR, Pei-Shih Chen, *Virginia Tech*

Influenza has been shown to be transmitted between nearby farms, but the potential for longer-distance transport, such as between cities or continents, is not known. A study of influenza virus concentrations in outdoor air has suggested that virus particles could be transported from mainland China to Taiwan. The goal of this research is to determine whether observed concentrations of influenza virus in Taiwan can be explained by transport over hundreds of kilometers coinciding with the occurrence of Asian dust storms that carry particles from central Asia toward the southeast. Using an atmospheric transport and dispersion model (HYSPLIT), we have examined back trajectories to identify likely source regions in China. To estimate a source strength, we synthesized information from the literature about the incidence rate of influenza and the amount of virus released by infected individuals. We then constructed simulations of virus transport from mainland China to Taiwan. Using a box model, we also estimated the local contribution to outdoor influenza virus concentrations. We have compared model results to measurements in Taiwan to estimate the contribution of transported vs. locally emitted influenza virus to the observations. This research is the first to assess the potential for atmospheric transport of influenza virus over hundreds of kilometers. Results from this research will help shed light on the epidemiology of influenza and may be used to inform policies aimed at reducing its spread.

7IB.3

Inactivation of Aerosolized Bacillus Anthracis Spores in the Vicinity of a Flame: Simulation Study. WORRAWIT NAKPAN, Michael Yermakov, Reshmi Indugula, Tiina Reponen, Sergey A. Grinshpun, *University of Cincinnati*

Survival of bio-warfare aerosol agents exposed to different, sometimes harsh environmental conditions, has gained substantial attention in the biodefense and biosecurity research communities. This basic simulation study aimed at assessing the survival of bacterial spores of *Bacillus anthracis* in the vicinity of a flame. The test conditions were intended to be relevant to a fire situation in a bio-weapon facility.

The survival of the aerosolized spores of *Bacillus thuringiensis var kurstaki* (Btk), a well-recognized surrogate of *B. anthracis*, was quantified after the spores passed a peripheral area of an air-acetylene flame in a close proximity. The flame type was chosen to represent a conservative situation since it has been demonstrated earlier that the combustion products of acetylene produce no biocidal effect on aerosolized Bacillus spores. The tests were conducted at two particle-to-flame proximity levels and seven exposure time intervals (ranging approximately from 0.1 to 6 s). The two flame positions corresponded to different weighted average temperatures in the exposure chamber, 170°C (precision=15°C) and 260°C (precision=25°C). The spores were tested at four air flow rates: 12, 18, 36, and 54 L/min. After passing the exposure chamber, the spores were collected on filters, removed into a liquid suspension, plated and subjected to a conventional culture-based analysis. Their survival was determined through comparison of the viability results obtained for exposed and non-exposed (control) samples. The aerosol concentration of viable spores in control experiments varied from one test to another ranging from ~10^6 to ~10^7 CFU/m^3.

At an exposure time ranging approximately from 0.1 s to 2 s, the survival fraction exponentially decreased as the exposure time increased. This held true for both temperature (proximity) conditions. Under the lower exposure temperature (greater distance to the flame), it was observed that the survival fraction decreased from 72% to 0.5%. It more drastically dropped at the higher temperature: from 60 to 0.015%. For both temperature (spore-to-flame proximity) conditions, the slopes noticeably changed once the exposure time exceeded ~2 s: the decrease of survival spores with the exposure time became slower. For the closer proximity condition, the limit of quantification (LOQ) in measuring the spore survival was in order of 0.002% so that the survival at a prolonged exposure was about to reach the LOQ. The same is anticipated for the greater proximity (the survival could likely reach the LOQ if the time was extended beyond the current 6-s upper testing limit).

In addition to the detection limitations of the experimental methodology used in this study, there may be an alternative explanation of the plateau in survival observed at the close flame proximity. The findings may point to a sub-population of spores that may have a particularly high stress resistance to the flame-originated heat. Existence of such a sub-population can be examined in a separate investigation.

The study results show that the aerosolized Bacillus spores traveling in the vicinity of a flame peripheral area may survive in appreciable quantities. This represents a great potential risk given a high chance that the viable agents remaining airborne can be subjected to a short- or long-range atmospheric transport. The findings justify the need of developing special materials with biocidal properties that can be deployed in such scenario to inactivate bioaerosol agents and consequently mitigate the risk.

This study was supported by the Defense Threat Reduction Agency (US Department of Defense).

7IB.4

The Effect of Humidity on the Viability of Aerosolised Bacterial Agents. EMMA KEYSER, Carwyn Davies, *DSTL*

In the event of an aerosol release of a biological agent, there is a need to understand the survival characteristics to evaluate the potential downwind impact. This is of vital importance for potential biological warfare agents, to assess the downwind hazard following release. To develop an understanding of the potential impact, it is necessary to investigate how different and varying environmental parameters can affect these aerosols. By altering these environmental parameters in a controlled laboratory environment, a full assessment of the survival characteristics of each pathogen can be determined.

Humidity is an important and variable factor that can have consequences on the stability and characteristics of a bioaerosol. Previous research, investigating the suspension of an aerosol over a prolonged period of time, has shown that relative humidity can affect the biological stability of a pathogen. Due to differing characteristics of individual pathogens, the impact of changing parameters, including humidity is likely to differ. For example, those pathogens that naturally thrive in wetter environments may benefit from higher levels of humidity, which may have a more detrimental impact on those that thrive naturally in relatively dry environments.

This study presents data showing the effects of different relative humidities on the stability and viability of a range of different pathogens contained within small particle aerosols over short distances and time from generation. Each pathogen was aerosolized at a range of humidities and evaluated using spray factor. Spray factor is one of the most effective ways of determining aerosol stability, and is calculated by taking the aerosol output and dividing it by the original concentration of the aerosol suspension. The spray factor was evaluated for a range of humidities for three different pathogens, including spore forming and vegetative cells.

7IB.5

Development of an Inhalational Francisella Tularensis Exposure Therapeutic Model in New Zealand White Rabbits.

ROY BARNEWALL, Chrs Cirimotich, Susan Reed, Kristin Patton, Heather Northup, Amber Lindsay, Phyllis Herr-Calomeni, Brian Miller, Gloria Sivko, *Battelle, Columbus Ohio*

Introduction

Tularemia, caused by the Gram-negative bacterium *Francisella tularensis*, is a zoonotic disease that causes a debilitating illness in humans. Human cases of tularemia are typically sporadic, with a primary concern around intentional release of the bacteria for biological warfare or bioterrorism purposes. Such an event would likely be attempted through aerosolization of the bacteria and result in primarily pneumonic tularemia, which is characterized by pneumonia, fever, chills, and other nonspecific symptoms. The natural incidence of *F. tularensis* in humans is too low to support clinical testing of new therapeutic countermeasures against the bacterium. Therefore, therapeutics will need to be tested under the US FDA Animal Rule and likely require two well-characterized animal models of pneumonic tularemia. To satisfy this requirement, a New Zealand White (NZW) rabbit inhalational tularemia therapeutic model was developed.

Materials and Methods

This model development was performed using NZW Rabbits in two phases: Phase I was performed to determine an inhaled median lethal dose (LD50) for *F. tularensis* Schu S4 and Phase II used the data generated under Phase I to develop an therapeutic model of lethal inhalation *F. tularensis* Schu S4 infection evaluating the efficacy of two classes of antibiotics, doxycycline (2.5 mg/kg, twice daily) and levofloxacin (50 mg/kg, once daily), when administered orally for 10 days after the onset of clinical illness in this model.

Phase I. 54 rabbits were challenged with varying doses of aerosolized *F. tularensis* (target 1 to 10,000 colony forming units (CFU)) and clinical observations were performed twice daily for 14 days for mortality. Blood samples for bacteremia analysis were collected from sedated animals (acepromazine; 1-6 mg/kg intramuscular) on days 3, 4, 5, 6, 7, and 14 post-challenge.

Phase II. 54 rabbits were randomized into 3 groups and challenged with a lethal dose of aerosolized *F. tularensis* to evaluate disease progression, including body weight and temperature, hematologic and clinical chemistry status, bacteremia status, mortality, and bacterial tissue burden for 14 days. It was determined a significant increase in body temperature (SIBT; two consecutive readings greater than two standard deviations above the average baseline temperature for an individual animal) was a suitable trigger for antibiotic treatment in this model. Thus, doxycycline (group 2) or levofloxacin (group 3) were administered after two consecutive SIBTs were detected for 10 consecutive days. Doxycycline was administered twice daily and levofloxacin once daily. All rabbits that died or were euthanized had necropsy and histology performed on select tissues to confirm death or illness due to tularemia. Samples of lung, liver, and spleen were collected for quantitative analysis of bacterial burden.

Results

Phase I Inhaled LD50 Determination. The calculated inhaled doses ranged from 4 to 24,168 CFU. The inhaled LD50 was calculated using a logistic model generated from the rabbit mortality data and was determined to be 266 CFU (95% Fieller interval: 120, 797).

Phase II. Rabbits were challenged with a mean inhaled dose of 4568 CFU of *F. tularensis* and were provided with antibiotics (doxycycline – Group 2; levofloxacin – Group 3) or no treatment (Group 1) following two consecutive SIBTs. Levofloxacin was completely protective against *F. tularensis* bacteremia, bacterial tissue burden, and tularemia-associated death, doxycycline was only partially protective with all but one animal succumbing and an average time to death of 266.4 ± 134.16 hours (11.1 ± 5.59 days). There were no survivors in the untreated controls with an average time to death of 138.41 ± 18.29 hours (5.76 ± 0.76 days).

Conclusion:

The results support the use of NZW rabbits as an animal model for evaluating therapeutic efficacy of candidate inhalational tularemia post-exposure countermeasures.

7IB.7

Insights into the Phenotypic and Virulence Differences Observed in Two Lineages of Burkholderia pseudomallei 1026b.

GREGORY WILLIAMS, Jeremy Boydston, John Yeager, David Dawson, Ryan Bartlett, Angelo Scorpio, Paul Dabisch, Ian Gut, *NBACC*

B. pseudomallei, the causative agent of melioidosis, is a highly adaptable soil dwelling organism which has a widespread distribution in equatorial regions of the world. This organism uses a vast repertoire of virulence factors to invade a host, evade immune responses, and establish an infection. Recent reports have demonstrated virulence differences among strains, and previous genomic comparisons have identified significant genetic rearrangement between highly virulent and attenuated strains/lineages. The present study demonstrated a significant difference in the virulence of two lineages of B. pseudomallei 1026b, namely Mahidol and NR-4074 from BEI Resources. The virulence of the NR-4074 lineage was significantly attenuated in a non-human primate model of inhalational disease. Additionally, these two lineages also had significant phenotypical and morphological differences when cultured at late stationary phase on different standard solid media. A genomic and transcriptomic comparison of these two lineages was conducted to examine potential genetic determinants of these phenotypic differences. These evaluations will provide information that can be used as the basis for future studies examining the genetic and regulatory mechanisms responsible for the large breadth of phenotypic diversity observed in this species.

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7IB.8

Influence of HVAC Operation on the Dissemination Pattern of Aerosolized Simulant Pathogen Particles in a Clinical Bio-Containment Unit. David Drewry, JENNIFER THERKORN, Thomas Pilholski, Gregory Bova, Kathryn Shaw-Saliba, Lauren Sauer, Brian Garibaldi, *Johns Hopkins University Applied Physics Laboratory*

The Johns Hopkins Hospital Bio-Containment Unit (BCU) is a state of the art facility to care for patients infected with high consequence pathogens, such as Ebola, SARS and multidrug resistant tuberculosis. Despite the high-risk nature of the work, there is currently limited guidance on the care of patients, emergency operating protocols and facility design for BCUs. Further, the role of air ventilation in the airborne transmission of nosocomial infection is still poorly understood. In this study, the influence of HVAC operating conditions on the dissemination of released pathogen particle simulants was investigated in the Johns Hopkins BCU. Test conditions included normal HVAC operation, and the loss of negative pressure during simulated HVAC exhaust failure. A suspension of optical brightener powder in water was nebulized by 3-Jet Collison Nebulizer to produce a polydispersed particle number size distribution ranging from 0.5-5 µm (i.e., simulant for droplet nuclei particles and a range representing high consequence airborne pathogens). The dissemination pattern and concentrations of the fluorescent particles were monitored by an array of eight fluorescent optical sensors (IBACs, FLIR Systems) located throughout selected areas of the BCU. During normal HVAC conditions, the released particles were contained in the patient isolation room with an average concentration of $1x10^4 \pm 3x10^3$ PPL, and a maximum peak concentration of $5x10^4$ PPL. Since there were no particles detected outside of the isolation room, this suggests that the locations and ventilation rates used by the patient room exhaust vents are sufficient to maintain airborne isolation conditions under static test conditions (i.e., with no healthcare workers or patient care activities conducted in the BCU). Under HVAC exhaust failure conditions, air flow in the patient room was reduced approximately 96% to 10 ± 3 CFM. Fluorescent tracer particles were detected in areas adjacent to the patient isolation room, including the personal protective equipment (PPE) doffing room and the main BCU corridor hallway. About 14% of the fluorescent particles detected in the patient room were transported into the doffing space. Since air movement with 1 m/s velocity was observed to flow in the direction out of the patient room through spaces around the door handles, it is hypothesized that particles were transported out of the isolation room via this route. Future research will further characterize the particle size dependent penetration factors through and around the patient room doors under different HVAC operating conditions (i.e., under different pressure differentials between the adjacent BCU rooms). Overall, this study provides a systematic method for evaluating airborne infection mitigation protocols in the BCU and suggests further steps to avoid healthcare worker exposure to high risk pathogens.

7IB.9

Disease Progression in African Green Monkeys Exposed to Small Particle Aerosolized Nipah Virus. MATTHEW LACKEMEYER, Lucy Cong, Michael Holbrook, Kyle Bohannon, Peter Jahrling, *NIAID*

Nipah virus (NIV) is a paramyxovirus that emerged in the late 1990s in Malaysia, with sporadic outbreaks extending into Bangladesh and India. Severe febrile response with respiratory and neurological disease is often associated with NIV infections in humans. Transmission can occur through direct contact, consumption of contaminated foods, and/or inhalational routes of exposure. Focusing on the inhalational route of exposure, most aerosolization studies involving infectious diseases utilize generated small particles (0.5-3.0 µm), which target the pulmonary region and deposit deep within the alveoli of the lower respiratory tract. Animal modeling involving nonhuman primates exposed to NIV is not well studied or characterized and no previous publications involving NIV involving aerosolization have been reported. Specifically, the NIV aerosol African green monkey animal model presented focuses on the disease progression and immune response generated from a small particle aerosol challenge to NIV. As expected, imaging analysis confirmed the deposited small particle aerosol was confined to the lower respiratory tract. Severe respiratory disease was observed with no overt neurological disease developing after exposure, which is not indicative of human disease. However, there was an increase in the cytokine response during the late stages of disease suggesting cell-mediated immunity. Further work is required to mitigate the severe respiratory distress caused from the aerosol exposure while extending the disease course and thus, increasing the potential for a neurological component often seen with the human disease condition. The goal of this study was to gain a better understanding of this disease progression, to observe any neurological distress that is associated with human NIV disease, and to evaluate the NIV nonhuman primate animal model for future development of medical countermeasures.

7IB.10

Host Transcriptomic Responses Predict Disease Severity in Nonhuman Primates Exposed to Small or Large Particle Aerosols Containing Burkholderia pseudomallei. JEREMY BOYDSTON, Adrian Caciula, Paul Dabisch, Xiaoyu Che, John Yeager, Jill Taylor, Gregory Williams, Ian Lipkin, Michael Hevey, Angela Rasmussen, *BNBI / DHS NBACC*

Burkholderia pseudomallei is a gram negative bacteria found in soil and water in Australia and Southeast Asia. Environmental exposure to B. pseudomallei, which may occur via percutaneous or inhalational exposure, results in the disease melioidosis. While the particle size distribution of naturally occurring aerosols containing B. pseudomallei has not been measured, measurements of naturally occurring aerosols containing other microorganisms suggest a wide range of particle sizes are possible. For many microorganisms, there is evidence that aerodynamic particle size is a significant factor influencing the disease presentation and lethality. Therefore, the aim of the present study was to examine the influence of aerodynamic particle size on the host transcriptional response to inhalational exposure of B. pseudomallei in nonhuman primates (NHPs). RNA-seq analysis of a time-series of blood samples revealed similar differential expression profiles independent of aerodynamic particle size. However, gene expression signatures were detected early in infection that allowed differentiation between NHPs that developed mild disease and those that developed severe or lethal disease. For example, activation of T-cells, specifically the T-helper 1 activation pathway involved in cell mediated immunity and macrophage activation, was significantly downregulated in NHPs that developed severe melioidosis, but not in those that developed mild disease. Such differences may be useful in the development of new prognostic assays. Transcriptomic signatures were also used to identify licensed drugs that are predicted to inhibit the expression profiles observed with severe disease, providing potential therapeutic candidates for future evaluation.

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All research was conducted in compliance with the Animal Welfare Act and other federal statutes and regulations relating to animals and experiments involving animals and adheres to principles stated in the Guide for the Care and Use of Laboratory Animals (National Research Council, 2011). The facility where this research was conducted is fully accredited by the Association for Assessment and Accreditation of Laboratory Animal Care International.

7IB.11

Evaluation of Ozone Efficiency to Reduce Airborne Virus Concentration in Ventilation Ducts. NATHALIE TURGEON, Jean-Gabriel Turgeon, Jonathan M. Vyskocil, Caroline Duchaine, *CRIUCPQ, Université Laval*

Over the last decades, the number of farm have decreased in North America in conjunction with an increase of the number of animal per farm. Disease transmission between animals in the same farm and also between nearby buildings is becoming a major concern in agricultural settings. Several bioconfinement and bioexclusion strategies have been proposed, such as air filtration. However, the installation of air filtration systems are expensive and require tremendous maintenance. Ozone concentration between 2.5 ppm and 3.5 ppm for 14 seconds was shown to be effective to obtain 99% reduction of infectious airborne viruses. However, theses concentrations are too high to be used in agricultural settings. The aim of this study is to design and validate a test duct to use ozone to reduce virus infectivity. Treatment of air in a test duct would allow contact of viruses with ozone without releasing ozone in the building, since ozone is destroyed before air exits the duct.

We assembled a ventilation duct of 220 m long with a 10 cm diameter to test several residence times and ozone concentrations. Air was driven through the duct at 0.6 m/s using an exhaust fan. Relative humidity inside the duct was adjusted to 40% and 80% using a humidifier located at tunnel entry. We used phage PhiX174 as a viral aerosol model. Phage aerosols were generated using a Collison 6-jet and injected into the duct after 150 cm. Aerosols were collected using All-Glass Impingers (AGI-30) after 0 minute residence time (150 cm after injection) as well as 1.5 minute, 3 minutes, and 6 minutes residence times. We tested ozone concentrations between 0.3 ppm and 1.8 ppm as well as residence in the duct without ozone. Air samples were analyzed using plaque assays. PhiX174 plaques obtained with ozone were compared with plaques obtained without ozone for the same residence time to assess the effect of ozone only. Ozone was more efficient at 80% RH compared to 40% RH to reduce PhiX174 plaque detection from air samples. With 6 minutes residence time at 0.3 ppm ozone we obtained 60% PhiX174 plaque reduction under 80% RH and 30% plaque reduction under 40% RH.

This communication describes the use of a test duct to measure ozone efficiency to reduce airborne culturable virus concentration. Reduction up to 60% of phage PhiX174 infectivity was obtained with 6 minutes contact with 0.3 ppm ozone. This technology could be used to test ozone treatment of exhaust air to prevent virus spread in agricultural settings.

7IB.12

Preliminary Evaluation of Commercial Bioaerosol Sampling Equipment in the Collection of Viable Aerosols of Clostridium difficile. CASEY COOPER, Kathleen Aithinne, David L. Johnson, *University of Oklahoma*

Airborne disseminations of Clostridium difficile (C. difficile) spores in healthcare environments have been documented in multiple studies and are potentially linked to the high transmissibility of healthcare acquired C. difficile infections. Effective air sampling methodologies are necessary to properly assess risks posed by C. difficile generation in healthcare facilities, but to date no studies have been performed to compare the efficiencies of commonly used bioaerosol sampling methods in collecting C. difficile spore aerosols. This laboratory study compared slit-to-agar impactor, liquid impinger, and filtration methods in the collection of laboratory-generated C. difficile spore aerosol.

Four air samplers evaluated in this study were the Airtrace slit-to-agar impactor, AGI-30 impinger, SKC BioSampler impinger, and a 47 mm MCE filter. Non-toxigenic C. difficile spores (ATCC 700057) were nebulized into a well-mixed polypropylene plastic enclosure operating under negative pressure and contained within a Class 2 biological safety cabinet. Side-by-side air samples were drawn from the chamber into the samplers in combinations of the Airtrace and the two phosphate buffered saline-filled impingers or the Airtrace and two 47 mm filter cassettes. A filter cassette was placed in line with each impinger to assess potential re-aerosolization. The Airtrace, previously used in published studies to collect airborne C. difficile spores, served as the reference method against which the other methods were compared.

Relative collection efficiencies of the two impingers were similar and were low compared to the slit-to-agar impactor. Filter cassette efficiency was higher than the slit-to-agar impactor. Impinger re-aerosolization of collected spores was low and somewhat higher in the AGI-30 than in the BioSampler, consistent with previous published studies using polystyrene latex spheres of a similar size.

This study is the first to compare the relative sampling efficiencies of four commonly used bioaerosol sampling methods when measuring C. difficile spore aerosol. The results demonstrate that the impinger bioaerosol samplers with phosphate buffered saline media were not effective in the viable collection of C. difficile spore aerosol, compared to either the slit-to-agar impactor or MCE filters. Additional research is needed to evaluate alternative and additional bioaerosol sampling methods for the collection of this important pathogen.

7IB.14

Identification of Toxic Mold Genes in Aerosolized Stachybotrys. Rhapsody Dearring, Qi Yao, Parisa Moghaddam-Taaheri, Amy Karlsson, AKUA ASA-AWUKU, *University of Maryland, College Park*

Indoor mold is a persistent problem that affects human health. Stachybotrys is the most common species of mold and is known to have toxic strains such as S. Chartarum. Not all airborne mold is toxic and thus the ability to identify toxic strains efficiently remains an issue. The specific focus of this project is to identify specific airborne strains of mold using aerosol science counting techniques and gene sequencing technology. Here we conduct experiments to determine efficient method of rapid quantification by varying concentrations of S. Chartrum. Furthermore, we also modify the time for deposition of the mold. The aerosolized concentrations are then deposited for subsequent analysis by Polymerase Chain Reaction (PCR). The novel method to analyze the airborne fungal strain is presented in detail. Gel electrophoresis is used to separate the DNA strands by size and the presence of the toxic mold gene, Tri5 is identified.

7IB.15

Surveillance and Detection of Influenza Viruses in Live Poultry Markets in Kunshan, China. Xinye Wang, EMILY BAILEY, William Lindsley, Gregory Gray, *Duke University*

Emerging respiratory viruses have led to considerable human and animal morbidity and mortality across China. Southeast and Eastern China in particular are considered hotspots for novel respiratory virus emergence as often dense populations of humans and domestic animals live in close proximity. There is also an additional risk of pathogen emergence associated with the continued use of live bird markets, where various species of live poultry are allowed to mix in close proximity. Birds are purchased and butchered onsite with little concern for potential human exposure or biosecurity. The goal of this study was to conduct bioaerosol sampling for influenza viruses in a local live bird market in Kunshan, China, a city of approximately 2.5 million individuals. Study personnel traveled to the bird market 2-4 times per week to collect bioaerosol samples over a 5 month period. Samples were collected using stationary 2-stage bioaerosol samplers provided by the National Institute for Occupational Safety and Health (NIOSH) connected to SKC AirChek Touch personal sampling pumps. Bioaerosol samples were chemically extracted and then processed by real time reverse transcriptase PCR for influenza A and B viruses. Of 153 bioaerosol samples, 39 were influenza A positive (cT value < 38), with no samples positive for influenza B. Initial results indicate that influenza A was circulating in live bird markets at high concentrations during the months of this study and in particular in the winter months, when most detections occurred (November to December). As current influenza concerns in Southeast Asia are related to emerging influenza A strains (H7N9, H5N1, etc.), this study demonstrates the need for additional surveillance at the human-animal interface in China. In particular, there is a need for additional research into the aerosolization of influenza viruses in open air markets, specifically bird markets, where large numbers of animals mix species and are in close contact with humans.

7IB.16

Concentration Profile of Influenza Virus in Day Care Centers. YU-CHUAN YEN, Yi-Lian Lee, Pei-Shih Chen, *Kaohsiung Medical University*

Day care attendance is considerable risk factor of influenza infection among children. Thus, early characterization for airborne influenza virus in high risk environment is of extreme importance. In addition, exhaled aerosol may carry airborne pathogens and play an important role for infectious diseases outbreak. Therefore, the purpose of present study in to investigate the airborne influenza virus of two day care centers with different ventilation system during four seasons, the air quality of two centers were also monitored simultaneously. Furthermore, influenza virus in exhaled air was also studied to understand the profiles of different disease status, and different host ag in this present study. To our knowledge, this is the first study regarding quantifying the concentration of airborne influenza virus in day care centers, either did assess influenza virus in exhaled air of infected children.

The concentration profile of airborne influenza virus was successfully characterized by filter with real-time qPCR assay in day care centers during Spring, Summer, Fall, and Winter, respectively. It was demonstrated that the positive rate of influenza virus in winter of two centers was significantly higher than other seasons, although the concentration of airborne influenza virus was significantly higher in summer due to the higher flu-like disease prevalence. In regard to the seasonal trend of other indoor pollutants, the concentration of total airborne cultivable bacteria and fungi was significantly higher in summer, but the concentration of carbon monoxide, carbon dioxide and number of ultra fine particle were highest in winter. In regard to the correlation between influenza virus and environmental factors, the positive rate of airborne influenza A virus and influenza B virus have an negative correlation with indoor temperature. In addition, it was also found out that the positive rate of influenza A virus and influenza B virus were all positively correlated with the concentration of indoor carbon monoxide regardless the difference of ventilation system. Furthermore, the concentration of airborne influenza A virus in both day care centers was positively correlated with the cold prevalence of children. In comparison with the Indoor Air Quality Recommended Values of Taiwan Environmental Protection Administration, the airborne cultivable bacteria concentration in both centers was 7－11 fold higher than the recommended value, and the failure rate of carbon monoxide and carbon dioxide was exceed fifty percentage.

An exhaled aerosol sampling device, developed in the present study, was demonstrated to provide an easy, noninvasive method to characterize the concentration of influenza virus in exhaled air. We have revealed the influenza virus could be exhaled during the latency period, and the concentration was increased when subject suffered cold symptom. It was also demonstrated that the older subject among five to six, the less virus could be exhaled. In addition, the concentration of influenza virus in exhaled air has a significantly positive correlation with the positive rate of airborne influenza virus.

In conclusion, we successfully demonstrated that the filter with real-time qPCR is a very sensitive and fast method to quantify airborne influenza virus in day care centers and in exhaled air of infected children. Airborne influenza virus was negatively correlated with temperature and positively correlated with carbon monoxide and other environmental factors were also investigated. In addition, airborne influenza virus was positively correlated with the number of infected children. Furthermore, profile of influenza virus during the whole disease period was also demonstrated.

7IB.17

Designed Micro-particles for Targeted Delivery of Anti-Tubercular Drugs. CHETHANI ATHUKORALA, Hema Priyamvada, CHETHANI ATHUKORALA, Hema Priyamvada, Shantanu Sur, Suresh Dhaniyala, *Clarkson University*

Treatment of pulmonary tuberculosis remains to be a major challenge, primarily due to the intracellular localization of tubercle bacilli inside macrophages and the ability of the bacteria to form a biofilm, both of which decreases the response to antitubercular drugs. Aerosolized delivery of antitubercular drugs has recently gained interest from its potential to effectively deliver the drugs into the affected lung regions without eliciting systemic side effects. We are working on the design of a core-shell microparticle formulation for antitubercular therapy deliverable via inhalational route: the biopolymer alginate core in these particles will allow a sustained release of DNAse to degrade DNA filaments in the biofilm; the shell consisted of self-assembled peptide nanofibers will enable the delivery of antitubercular drugs and macrophage targeting. A tetrapeptide tuftsin epitope will be presented on these nanofibers to promote macrophage targeting and particle internalization, while anti-tubercular drug isoniazid conjugated to the peptide through hydrazine linkage will allow the release of drug at the target site. The details of our approach using nebulization and electrospray techniques to optimally generate these therapeutic particles in the targeted size range of 1 – 3 µm will be presented. We are currently investigating the release of DNAse from these microparticles and their interaction with macrophage cell line. Our strategy of combining in a single microparticle the delivery of antitubercular drugs, macrophage targeting, and biofilm degradation capability could allow for the development of an efficient therapy for pulmonary tuberculosis.

Keywords: Core-shell microparticles, aerosol therapy, pulmonary drug delivery, tuberculosis therapy

7IB.18

Antibiotic Resistance Genes Spread via Exhaled Breath. YUNHAO ZHENG, Jing Li, Xinyue Li, Maosheng Yao, *Peking University*

Antibiotic Resistance Genes (ARGs) recently draw a global attention. The increasing usage of antibiotics drugs leads to the emerging of antibiotic resistant bacteria and antibiotic resistant genes (ARGs). In a previous study, Methicillin-resistant Stphylococcus aureus (MRSA) was detected from exhaled breath. Here, we further used the dBLueTech BioScreen device to collect the EBC samples from human subjects with respiratory tract diseases, including chronic obstructive pulmonary disease (COPD) , upper respiratory tract infection(URTI), and healthy people. And then we screened relative abundances of 39 ARG subtypes resistant to 7 common classes of antibiotics including quinolones, β-lactams, and macrolides in the EBC samples. Besides, bacterial communities were also profiled using 16S gene sequencing on the Illumina MiSeq platform. Results showed that the relative abundances of ARGs in URTI patients were higher than those of COPD patients and healthy people. Resistance gene of qepA to quinolone was found to be the most abundant in the exhaled breath, followed by blaTEM to β-lactam. By combining with high throughput gene sequencing, we found that respiratory infections exhibited significant impacts on the structures of microbial communities in the respiratory system. The results from this work also indicated that these ARGs and pathogens could be emitted and transmitted through the exhaled breath, thus adding to additional risks of infectious disease transmission. These data also suggest that people, even in healthy state, are carriers and transmitters of ARGs, exhibiting far more influences than currently understood.

7IB.19

Viability of Aerosolized Murine Noroviruses in Experimental Setup. MALIN ALSVED, Anders Widell, Mats Bohgard, Patrik Medstrand, Jakob Löndahl, *Lund University, Sweden*

Introduction
Norovirus is the major cause of acute gastroenteritis in the world and it is considered to spread by food, contact, by the fecal–oral route and by droplets from splashes. However, there are studies showing disease transmission between individuals without contact, indicating airborne transmission [1]. One previous study successfully detected NoV RNA in air samples from hospitals [2]. However, important issues that remain to be understood are for instance what sources that generate airborne NoV and to what extent airborne NoV are infectious.

In order to understand what parameters that affect the infectivity of airborne NoV, we have developed an experimental setup for aerosolization and collection of murine noroviruses (MNV), a cultivable model virus for human NoV.

The genomes of NoV and MNV are of positive sense strand RNA. During replication, the intermediary, complementary minus strand RNA is formed inside the infected cells. By specifically detecting the minus strand RNA in cells, infection can be identified with high sensitivity and specificity [3].

Methodology
MNVs in cell culture medium were aerosolized by an atomizer (Model 3076, TSI inc.) into a 1 m long stainless steel flow tube, and collected at the end of the flow tube into phosphate buffer saline (PBS, Life Technologies) solution with a BioSampler® impinger (SKC inc.). The particle number concentration and size distribution of the aerosol was monitored by a scanning mobility particle sizer (SMPS, built in-house, Lund University) and an aerodynamic particle sizer (APS, Model 3321, TSI inc.).

The liquid in the BioSampler® was analyzed by reverse transcriptase quantitative polymerase chain reaction (RT-qPCR) targeting the viral genome (positive RNA) to determine the number of collected viral RNA genomes. For infectivity analysis, inoculation of the collection liquid on RAW 264.74 cells was performed during 72 h. After the incubation time, the cells and the supernatant were separated for analysis. Intra and extracellular RNA was obtained by RNeasy Mini Kit (Qiagen) and detected by strand specific plus and minus RT-qPCR as described by Vashist et al. [3].

Results and Discussion
The aerosolized and collected MNV that were inoculated on cell cultures showed cytopathic effect (CPE) on the cells by visual observation in a microscope. Infections were confirmed by the minus RNA RT-qPCR analysis on the cells after the incubation time. The lower limit of detection of minus RNA was 10^2 genomes/mL and the concentrations of intracellular minus RNA after incubation were in the range of $1.5 \cdot 10^3$ to $3.9 \cdot 10^6$ genomes/mL. This infectivity assay, thus serves as a sensitive qualitative determination of MNV infection. This is useful since visual CPE observations need a trained observer to be correctly analyzed. Our future goal is to develop the assay to give relative quantitative information on virus infectivity.

Conclusions
In this study we have successfully developed a setup for experimental studies on airborne MNV. From our results, we saw that infectivity was preserved after aerosolization. This experimental setup allows further studies to be made to gain insight into what factors that affect infectivity of airborne MNV.

Acknowledgements
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7IB.20

Development of an Inhalational Animal Model of Q Fever. SARA RUIZ, Aysegul Nalca, *US Army Medical Research Institute of Infectious Diseases*

Until recently, *Coxiella burnetii* research was hampered by its obligate intracellular nature and inability to be propagated outside of mammalian cells. With the advent of an axenic growth system, many avenues are now able to be pursued. Characterization of the bacterial stock is essential prior to utilization in animal experimentation. Four strains of *C. burnetii* (Nine Mile, Q229-K, RSA334, and Henzerling) were examined for viability, purity, and morphology. Due to the robust growth of Nine Mile in comparison to the other strains, it was chosen as the best candidate to proceed with for future studies. Sham aerosols were performed and demonstrated the ability to deliver aerosolized *C. burnetii* with particles with a mass median diameter capable of depositing in the lower airways across numerous species. A comparative study between A/J and C57Bl/6 mice demonstrated that all aerosol challenged mice had clinical signs to include weight loss and temperature changes. Bacterial DNA was recovered in the lung, liver and spleen with the highest burden reported in the spleen. Cynomolgus macaques were found to be a sensitive model in which all challenged animals developed a dose dependent respiratory illness. Lethal disease was induced in animals receiving the highest dose. Future experimentation is building upon the foundation of the characterization work to develop an inhalational non-human primate model of Q fever for future medical countermeasure screening.

7IB.21

B. anthracis Spore Persistence Following Aerosol Challenge in New Zealand White Rabbits. SARA RUIZ, Aysegul Nalca, *US Army Medical Research Institute of Infectious Diseases*

Bacillus anthracis spore persistence has been well documented in human clinical cases and animal models of disease. The underlying mechanism of spore persistence has yet to be elucidated although is likely due to an interplay between host immunological factors and bacterial virulence determinants. New Zealand white rabbits were challenged via aerosol with *B. anthracis* at a uniformly lethal dose followed by treatment. A subset of experimental animals were euthanized at one and 24 hour post-exposure to ascertain lung deposition and dissemination. Challenged animals were monitored 90 days post-exposure for clinical signs of disease to include respiratory rates, activity level and general appearance. Lung, spleen and lymph node tissue was recovered when an animal was found moribund or at end of study to assess spore persistence following treatment and apparent resolution of disease. This study will establish a model in which to correlate differing treatment regiments and spore persistence in an inhalational model.

7IB.22

Strategies for the Deployment of a Bioaerosol Air Sampling Network Following a Wide Area Attack. JONATHAN THORNBURG, Paul Mobley, Jean Kim, Prakash Doraiswamy, Timothy Boe, John Archer, M. Worth Calfee, Leroy Mickelsen, Sang Don Lee, *RTI International*

Following the wide area release of a biological agent, like *Bacillus anthracis*, one source of uncertainty confronting decision makers is the degree to which reaerosolized organisms present a public health hazard. Bioaerosol sampling methods deployed as individual samplers or as an integrated network may provide federal agencies, like the U.S. Environmental Protection Agency, another option for responding to a wide area biological incident. This study assessed whether a bioaerosol sampling network could cost-effectively detect spores reaerosolized from urban surfaces.

We performed the air sampling network assessment in two phases. Both phases incorporated publicly available information on bioaerosol sampler performance, spore emission rates, meteorology, and estimated cost. The first phase used Excel models to assess the types of bioaerosol samplers that should be considered for the more detailed assessment. In the second phase, we developed a system performance model (SPM) in MATLAB to optimize the bioaerosol sampling network design for detection probability and minimize cost. We evaluated four different bioaerosol network strategies deployed in two cities, Denver, CO and New York City.

Phase 1 results determined that current commercially available point and stand-off, real-time bioaerosol sensors do not have the sensitivity to detect resuspended spores. Calculated bioaerosol concentrations, even near the point of resuspension, were always less than 1000 agent containing particles per liter. Therefore, we developed four bioaerosol network strategies based on 1) low flow filter samplers, 2) high flow filter samplers, 3) native samples like building ventilation filters, and 4) a combination of the three. Preliminary Phase 2 results using the SPM found that a ratio of 1:4 high flow to low flow samplers, 80 total, detected bioaerosol concentrations less than 10 colony forming units per cubic meter for up to 30 days following an attack. A significantly higher density network comprised solely high flow or low flow samplers provided equivalent detection capability but also doubled the period of detection. These results were based on a limited range of spore resuspension rates, human activity levels, and meteorological conditions. Further work will expand the range of data inputs and include strategy 3. The outcome will be an optimized network design for each city to provide the highest probability of bioaerosol detection for the maximum time period balanced against the cost of the network.

7IB.23

Aerosol Sampler Selection Impacts Quantification of Viable Burkholderia Pseudomallei. JILL TAYLOR, Michael Schuit, Paul Dabisch, *BNBI / DHS NBACC*

Burkholderia pseudomallei is a Gram negative bacteria found in soil and water in Northern Australia and Southeast Asia. B. pseudomallei has been detected in outdoor aerosols associated with specific contamination sources and down-wind cases of melioidosis, suggesting that inhalation of naturally-occurring aerosols containing the bacterium is a likely route of exposure. Previous field and laboratory studies have utilized both all-glass impingers and gelatin filters to measure viable airborne bacteria. However, it is known that aerosol samplers vary with respect to their ability to preserve the viability of collected microorganisms, depending on the relative resistance of the organisms to impaction, desiccation, or other stresses incurred during the sampling process. Therefore, to maximize the chance of detecting viable microorganisms in a field-sampling setting, it is critical to appropriately match the sampler to its target. The aim of the present study was to assess the performance of multiple commonly utilized aerosol samplers for sampling airborne B. pseudomallei, specifically the all-glass impinger, gelatin filter, midget impinger, and Mercer cascade impactor. Aerosolized B. pseudomallei was sampled with all four sampler types simultaneously. Preliminary results demonstrate that the average physical sampling efficiency, assessed using 1 µm fluorescent polystyrene beads in growth media, was significantly lower for the midget impinger when compared to the other samplers. Smaller, yet statistically significant differences between some of the other samplers were also noted. Additional testing to assess the biological sampling efficiency has been performed and results will be discussed. The results of the present study are useful to inform future studies in which the quantification of infectious airborne bacteria are necessary for exposure and risk assessment.

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7IB.24

Modeling the Aerobiologic Transmission of Tuberculosis: Aerosol Studies using the Nonhuman Primate. RACHEL REDMANN, Stephanie Killeen, Nadia Golden, Deepak Kaushal, Chad J. Roy, *Tulane University*

Tuberculosis is an aerosol-acquired pulmonary disease that is caused by exposure to and infection with *Mycobacterium tuberculosis* (*Mtb*). Transmission occurs primarily through effective transfer of bacilli-laden respiratory secretions from an infected to naïve host. Tubercular disease is commonly studied using experimental infection in animas that include the rabbit and nonhuman primate. The latter species is considered to be a near-clinical animal model of active pulmonary tuberculosis and is an optimal test system for studying transmission phenomena. The rhesus macaque (*Macaca mulatta*) represents a highly refined model of clinical tuberculosis, with development of active pulmonary disease that shares remarkable similarities to clinical tuberculosis in humans. The rhesus was subsequently utilized to study transmission and was experimentally aerosol-infected with two strains of *Mtb* of varying virulence (str. *Erdman* or *CDC1551*). Prior to aerosol infection, strain-specific aerosol susceptibility was determined in order to understand environmental survival of laboratory-generated bacilli and to properly target low-dose aerosol animal infection. The *Erdman* strain of Mtb approximated the comparator low virulence strain *CDC1551*, with a mean spray factor within 1 log (*Erdman*: 4.0E-07±2.3E-06; *CDC1551*; 9.0E-06±6.7E-06). Thereafter, rhesus macaques (n=8) were experimentally infected by small particle aerosol exposure (MMAD=1 µm; σ_g=1.4) with either *Erdman* or *CDC1551 Mtb* each at a target inhaled dose of 250 CFU. Animals were monitored for development of disease over the next 12 weeks, including biological outcome parameters correlative with development of disease (e.g., PPD positivity, C reactive protein, radiographs, presence of bacilli in lavage fluid). Animals were monitored for development of physiological changes, specifically in their exhaled breath throughout the study. Sampling included semi-continuous monitoring of ambient air within specialized input-only HEPA-filtered sealed primate caging units, and weekly face mask-based collection of exhaled breath during physical examination. In addition, respiratory function was measured using whole-body plethysmography. Aerosol parameters measured within the caging units and face masks included cumulative (total) particle counts and distribution-specific data collection. Aerosol samples were also collected using size-selective filters (0.3 µm; 37 mm MCE) in both configurations which were subsequently eluted in media (LB) and cultured for presence of Mtb; split samples were also subjected to PCR for Mtb genomic material. Results showed animals experimentally infected with the virulent strain (*Erdman*) experienced rapid development of active pulmonary tuberculosis, with a mean of 5-6 weeks before recommended euthanasia. This outcome contrasted to *CDC1551*-exposed animals, which developed disease at a gradual tempo, averaging 10-12 weeks before termination of study. Physiological changes, specifically respiratory measurements via plethysmography, was largely determinative of the strain of *Mtb* used for experimental infection. Minute volume (V_m) and frequency (f) doubled within 2-3 weeks of infection in *Erdman*-infected animals contrasting to *CDC1551* animals where similar changes were observed 4-5 weeks post experimental infection. Aerosol monitoring showed a peak in total particles (≈7.0E+06 particles/20 liters) in Erdman-exposed animals at week 4 post-infection whereas particle production peaked in *CDC1551*-exposed cohorts at week 7-8 post-infection. The distribution of particles collected during infection markedly changed as the disease severity and tempo intensified, with the respirable fraction of particles produced increasing upon culmination of disease across both strains of *Mtb* used for infection. This study is one of the first to attempt to measure exhaled breath aerosol production during experimental infection with *Mtb* using a species that produces a near-clinical model of tubercular disease. This approach provides a basis to determine and characterize initiation and production of *Mtb* in respiratory secretions in the context of tuberculosis disease and represents an expert system by which to study infectious transmission.

7IB.25

Characterization of Aerosolized Middle East Respiratory Syndrome Coronavirus Infection in African Green Monkey Model. Allison Totura, Virginia Livingston, Ondraya Frick, David Dyer, AYSEGUL NALCA, *USAMRIID*

Middle East respiratory syndrome coronavirus (MERS-CoV) was first identified as a cause of a lethal respiratory disease outbreak in Saudi Arabia in 2012. MERS-CoV has caused isolated outbreaks in Saudi Arabia since 2012 with 483 deaths (40% mortality rate). On May 20, 2015, the first case outside of Saudi Arabia was reported in South Korea and resulted in a major outbreak with 179 confirmed cases and 29 fatalities. Although it is thought that animals, especially camels and bats, are the most likely reservoirs of MERS-CoV in nature, the exact routes of transmission and the role of these animals in transmission are still unknown. Clinical signs of disease in humans range from asymptomatic to severe acute respiratory syndrome and death. Typically fever, cough and shortness of breath are observed in patients, but pneumonia is not always present. Gastrointestinal abnormities, such as diarrhea, and acute renal failure have also been observed in these patients. Although there are several animal models developed by using different routes of infection, there is not any animal model that truly emulates the human disease. In this study, twelve African green monkeys (AGMs) exposed to high, mid and low target doses of aerosolized MERS-CoV. Disease progression was followed with daily observations, weights, body temperatures, blood and throat swab collections. Data indicated that disease severity was dose dependent and all the AGMs survived the disease.

7IB.26

Downstream Effects of Ameobic Co-culture on B. pseudomallei. SARA RUIZ, Katie Beck, Aysegul Nalca, *US Army Medical Research Institute of Infectious Diseases*

Burkholderia pseudomallei, the etiological agent responsible for melioidosis, is able to persist within water and soil of endemic regions. Human infection occurs through direct exposure to the contaminated environment via oral or respiratory routes. The mechanism through which *B. pseudomallei* persists within the environment is a critical gap in the field's knowledge. Free living amoeba have been shown to provide a protective niche for other environmental bacteria. The interaction between *Acanthamoeba* and *Legionella pneumophila* allows for a protected replication site, and has been observed to create a more successful bacterial pathogen, increasing its virulence through an unknown mechanism. *B. pseudomallei* is known to survive within the free living amoeba, *Acanthamoeba astronyxis*. The downstream effects of amoebic passage on *B. pseudomallei* were investigated. *B. pseudomallei* was found to replicate more efficiently upon co-culture with amoeba than grown in media alone. The resulting bacteria from the amoeba co-culture infected mammalian cells at a statistically significant higher rate. Aerodynamic properties for both passaged and non-passaged bacterial populations are being assessed. Environmental sampling is dependent upon understanding the niche in which the bacteria lives. The effects of co-culturing amoeba and *B. pseudomallei* potentially has a direct relationship to predicting outbreaks and identifying populations most at risk for infection. In addition, novel medical countermeasure targets could be identified through the transcriptomic analysis.

7IM.2

Signal Detection for the Measurement of Aerosol Scattering Coefficients with an Integrating Nephelometer. HANS MOOSMULLER, Herbert Schloesser, *Desert Research Institute*

Integrating nephelometers measure aerosol scattering coefficients integrated over most scattering angles (~4π) and generally detect and quantify the scattered light with photon-counting photomultipliers. Most commercial nephelometers use a background-subtraction scheme, measuring sequentially the scattering signal with the nephelometer light source turned on and the background signal with the light source turned off, and subtracting the background signal from the scattering signal. This scheme can be problematic for fast changing aerosol concentrations such as encountered in airborne applications near or in aerosol plumes. Such problems are exacerbated for multi-wavelength operation.

Here, we investigate different signal detection schemes for photon-counting nephelometers, including a detailed comparison of background-subtraction and Fourier-transform methods. Our signal analysis is based on the Poisson statistics of the photon-counting signal, simulating different detection schemes for single and multiple-wavelength nephelometers.

7IM.3

Enabling Long-Term Operation of a Motion-Tolerant, Water-Based Condensation Particle Counter. STEVEN SPIELMAN, Gregory Lewis, Nathan Kreisberg, Susanne Hering, *Aerosol Dynamics Inc.*

The International Space Station presents a unique challenge for monitoring the particulate air quality to which astronauts are exposed. Sensors must be small, operate at near zero-gravity, and yet be capable of long-term operation. Other applications, such as personal monitoring, require tolerance to tipping and jarring, which imposes similar limitations on the instrument design. While optical and electrometer-based sensors generally meet the requirements of motion-tolerance, zero-gravity, long-term operation, this is not the case for condensation particle counters.

Previously we introduced motion-tolerant, a self-sustaining, water-based condensation particle counter. Called MAGIC, for moderated aerosol growth with internal water cycling, this instrument has no internal water reservoirs, and thus tolerates tipping and jarring, yet operates for days to weeks on a single charge of the wick. Using the “moderated” water condensation growth tube approach, water vapor from the heated, wet-walled condensation section is captured by the wick in the cooled downstream section. Sustained operation is accomplished through a combination of extraction of additional water from the sampled air stream, and internal capture of water vapor by the wick. Because there are no exposed liquid reservoirs, the instrument can be operated in any orientation, or under zero-gravity.

Presented here is the adaption of MAGIC to long-term operation, with the aim of providing many months of continuous operation. Key developments are a (1) wick moisture sensor to enable direct control of the wick water, and (2) a new dead time correction method which allows use of a wider, and more robust focusing nozzle without loss of high particle concentration measurements.

The wick moisture sensor uses an optical sensor to assess the wick transparency. Because the wick material is a porous structure with a fine (sub-10 µm) pore size, it scatters light when dry. When wet, the pores fill with water and it becomes translucent. We inserted a dark material under the outer layer of the wick to creates a structure that darkens when wet. The sensor measures the reflected light to generate a signal that varies with moisture content. Tests under conditions in which the wick is slowly dried demonstrate that the sensor shows deviation from a fully wetted state well in advance of the loss of instrument performance. Coupled with an algorithm to control the temperature of the water-recovery stage, this provides a direct, verifiable means to ensure long-term maintenance of a properly wetted wick.

The second change focused on development of a droplet detector that is less sensitive to optical alignment. This in turn leads to longer light scattering pulses for individual droplet, and hence a higher rate of coincidence for the same particle concentration. As in many condensation particle counters, we directly measure fraction of time during which the scattered light signal is above the threshold, and therefore unable to distinguish an incoming, coincident pulse. Yet, because of the finite threshold and overlapping tails of neighboring pulses, this measured time is longer than the effective dead time. For years condensation particle counters have estimated the effective dead time by multiplying the measured dead time by an empirical dead time correction factor. However, at very large dead times this approach over-corrects. Presented here is an alternative approach that provides accurate counting when measured dead times are in excess of 90%.

7IM.4

Numerical Simulation of a Parallel-plate Separator for PM2.5. TAKUTO YONEMICHI, Koji Fukagata, Kentaro Fujioka, Tomoaki Okuda, *Keio University*

Particulate matter suspended in air such as PM2.5 has adverse effects on human health by depositing on respiratory tracts. Measurement of charging states of PM2.5 and charge distribution of ambient aerosol have been carried out because charged particles deposit on the respiratory tracts more than non-charged particles. Okuda et al. (2015) developed a parallel plate particle separator (PPPS) in order to classify PM2.5 for measurement of charging state of individual particles. The PPPS consists of three sections: the inlet section, classification section, and exit section. The inlet section consists of three conduits. Particles are introduced from the central conduit, whereas clean air is supplied from the other two. When the particles flow in the classification section, they are moved toward the electrodes by the Coulomb force. Finally, they are classified by their charging states at the exit section consisting of three conduits similar to the inlet section. However, this device has uncertainty in classification performance: some particles flow out to unexpected exits. Therefore, improvement of this performance is needed for a more accurate measurement.

In the present study, dispersion of submicron particles in the PPPS is numerically analyzed by means of the Lagrangian particle tracking method including a model of the Brownian diffusion in order to reveal the mechanisms of the classification uncertainty. Further, a parametric study is made in order to find the optimal condition which decreases the classification uncertainty.

The results show that 7.5% of total particles flow out to the unexpected exits due to the Brownian diffusion. Decreasing flow rate of the central inlet for aerosol and increasing flow rate of the other inlets for clean air dramatically improves the classification performance. The outflow of particles to the unexpected exits becomes 0.0% when the flow rate of the aerosol is less than 84% compared to that in the base case. This improvement is in good agreement with experimental observation. In addition, it is found that similar improvement can be attained by narrowing the central inlet.

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7IM.5

Measurement of Effective Density of Submicron-sized Ambient Aerosols Using a Lab-made Single Stage Low-pressure Impactor with Scanning Mobility Particle Sizer. JANG-SEOP HAN, Junho Hyun, Jungho Hwang, *Yonsei University, Korea*

The structure of particles is directly related to their transport properties and plays an important role in determining their deposition pattern in the human respiratory system. Previous studies report that agglomerate particles can deposit on human lung more easily than spherical particles since the specific surface area of the agglomerate particles is larger than that of spherical particles (Morawska et al., 2005; Scheckman and McMurry, 2011). The particle effective density is a parameter that describes the combined effects of particle density and shape upon aerosol motion.

To measure the particle effective density, it is typical to use two instruments connected in series. Kelly and McMurry (1992) introduced a basic approach used in this methods and utilized this technique to analyze lab-generated particles. They used a differential mobility analyzer (DMA) and a microorifice uniform deposit impactor (MOUDI) with known cutoff diameters. To measure the effective density of DEPs, Maricq and Xu (2004) and Van Gulijk et al. (2004) used an electrical low-pressure impactor (ELPI). In their works, DEPs were classified by DMA, then brought to ELPI with which the aerodynamic diameter of DEPs was measured.
Park et al. (2003) also used a DMA but they used an aerosol particle mass analyzer (APM) instead of ELPI. For each APM voltage, the particle number concentration was measured with a condensation particle counter (CPC), and the peak APM voltage, which corresponds to the peak mass for the mobility-selected particles, was determined. The particle effective density was obtained by carrying out sequential measurements on DEPs and polystyrene latex (PSL) spheres of the same mobility size.

In this paper, a new methodology was developed by using a low-pressure impactor and SMPS to obtain the effective density of ambient aerosol particles. The low-pressure impactor, a corona charger and aerosol electrometer was used for the electrical current, and SMPS measured the size distribution of the aerosol. The mobility diameter measured from SMPS was changed into aerodynamic diameter with assumed effective density, then the number concentration was estimated using efficiency of the impactor. The currents were calculated with the estimated number concentration and compared with the measured value. The methodology was validated with lab-generated sodium chloride (NaCl) particle then the effective density was obtained from various places.

Outdoor particles had similar effective density about 0.81 to 0.91. Indoor aerosols had different effective densities – 1.83 for the office A, 0.6 for the office B, 0.69 for the house, 1.06 for the underground parking lot. The size distributions of particles in the office and the house were similar and the effective density were also similar. The geometric mean mobility diameter of particle in the underground parking lot is 25.8 nm. The main source of the underground parking lot is the vehicle exhaust gas. The effective density and size distribution of the office A was very distinct from other places because nanoparticle experiment was performed in this office.

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7IM.6

Calibration of Particle Number Concentration by Mobility-based Particle Size Distribution Instruments with Metrological Traceability. YOSHIKO MURASHIMA, Hiromu Sakurai, *AIST*

Particle size distribution (PSD) measurements based on electrical mobility classification can accurately measure particle size and number concentration of fine particles and are used for various applications. Performance evaluation methods for them, however, have not been established, especially for particle number concentration. For conventional scanning mobility particle sizer (SMPS) spectrometers that consist of separable components accessible to the user, the performance can be evaluated to some extent by individually inspecting and/or calibrating the components such as the charger, classifier, and detector. On the other hand, the fast-response instruments such as TSI's fast mobility particle sizer (FMPS) are packaged so that the integrated components are not separable for individual testing. The same can be said for recent compact, battery-powered portable instruments. For those instruments, techniques to evaluate the overall performance of a complete system as a whole are needed by treating each instrument as a "black box". Such techniques would be also useful for testing conventional SMPS's in addition to the tests/calibrations of individual components. This method also allows evaluation of the performance of a charger in a conventional SMPS in terms of the extrinsic charging probability.

We propose a method that evaluates the overall performance of a particle size distribution measurement based on checking the accuracy of the total number concentration using monodisperse particles such as polystyrene latex (PSL). In this method, the total number concentration of monodisperse particles of the same aerosol is measured in parallel by a test PSD instrument (e.g., SMPS) and a reference CPC. The total number concentration that is determined by integrating the size distribution density function measured by the test PSD instrument ($C_{N,test}$) is compared with the number concentration measured by the reference CPC ($C_{N,ref}$). Monodisperse particles are generated by passing particles from an aerosol generator (e.g., electrospray) through a neutralizer and subsequently classifying them with a differential mobility analyzer (DMA). Then, after mixed well with a dilution air, particles are delivered to the test PSD instrument and reference CPC simultaneously. By using a reference CPC that has been calibrated with traceability to a national or international standard (e.g., AIST's primary standard), the test PSD instrument calibrated by this method will have metrological traceability to the standards with respect to particle number concentration.

We applied this method to two commercial instruments, which were a TSI SMPS model 3936L75 with an Am-241 neutralizer separately installed and without an impactor, and a TSI engine exhaust particle sizer (EEPS) spectrometer model 3090. Monodisperse PSL particles of 4 sizes (particle diameter: 30, 60, 100, and 200 nm) were used, and a total number concentration measured by the test PSD instruments was compared to the value by calibrated CPCs in this evaluation. We will report the results and discuss the uncertainties of the evaluation. We found that, while the information obtained in the tests was somewhat limited, the method was simple to perform and allowed size-resolved and quantitative evaluations of the performance of the test instruments, which would be useful for example in determining size-dependent correction factors and identifying malfunctioning components, even for a black-box instrument.

7IM.7

Measurement of Continuous PM and Black Carbon in a Wood Stove Dilution Tunnel. GEORGE ALLEN, Lisa Rector, *NESCAUM*

The US EPA 2015 New Source Performance Standard (NSPS) for residential wood heaters includes development of test method protocols that use cordwood in lieu of the traditional dimensional lumber fuel for PM emission performance certification. This move to new fuels focused the need to improve the operational component of the EPA M28R test protocol for wood stoves. Both the process of designing a new test fueling protocol as well as a better understanding of how stove design needs to be changed to reliably burn cordwood cleanly can benefit from highly time-resolved measurement of aerosol emissions to identify what fueling and operational conditions dominate the emission test results. As part of several ongoing projects to inform upcoming Step 2 cordwood test protocols for the 2015 NSPS, robust techniques to measure continuous PM in a dilution tunnel have been developed. The Thermo 1400AB and 1405 TEOM ambient PM monitors have been operationally modified to provide robust 15-second PM measurements for this application, and are capable of measuring in excess of 1/2 gram/m^3 PM. TEOM filter changes are typically 30 to 120 minutes or more apart and result in a data gap of only 2 to 3 minutes; a typical test for a clean technology stove usually has only a single filter change. Comparison to Method 5G manual filter PM samples shows high correlation over a wide range of concentrations and good numerical agreement. No sample conditioning is used for TEOM measurements. The TEOM uses the same Emfab TX40 filter media as the Method 5G sample trains, is run at the same temperature (30C), and with a similar face velocity. While semi-volatile (water, SVOC) mass dynamics are present in the TEOM data, because filter conditions are the same, they are the same dynamics occurring on the Method 5G samples. The only functional difference between the methods is that the TEOM filters can not be equilibrated using the required Method 5G filter desiccation process. TEOM data often go negative when filter loading is high and the burn cleans up; for fresh woodsmoke this is more likely due to SVOC loss than water, and more research is planned to quantify the components of this mass loss. A Thermo pDR1500 forward scattering particle instrument is also used to provide supporting PM measurements as well as a qualitative indication of particle size from the ratio of TEOM to pDR concentrations, since the pDR response to PM varies widely across the range of burn conditions during a test cycle. For a subset of test runs, black carbon (BC) is also measured in the dilution tunnel using an operationally modified Magee Scientific AE22 Aethalometer. Using a manual tape advance approach, 5-second BC concentrations in excess of 20 milligrams/cubic meter can be measured, with a data gap of 5-seconds between tape advances. The "gap" method is used to estimate and correct for filter optical loading artifacts. Measurement of continuous PM and BC provides a real-time estimate of the organic carbon (OC) aerosol mass (by difference) and thus the BC to OC ratio, which can be indicators of combustion conditions. Future work includes plans to perform the required EPA method testing to allow the TEOM to be used as an alternative to the current manual measurements for PM emission performance certification of residential wood heaters, and to couple the TEOM with a commercial dilution system to provide an alternative to the current dilution tunnel emission measurement approach.

7IM.9

Characterization of a Dimer Preparation Method for Nanoscale Aerosol. NICHOLAS ROTHFUSS, Sarah Suda Petters, Markus Petters, *North Carolina State University*

The synthesis of nanoscale aerosol dimers by charge-assisted particle coagulation is a technique suited for a variety of applications that are just beginning to be explored. Here we build upon the approach of Rothfuss and M. Petters (Aerosol Sci. Technol. 50(12), 2016), which has been implemented for the measurement of particle phase state. Dimer particle morphologies are prepared by coagulation of mobility selected particles carrying opposite charges. Coagulated charge-neutral dimers can subsequently be isolated by electrostatic filtration and used in studies that exploit the unique particle morphology to study aerosol properties. The nanoscale dimers are differentiated by their electrical mobility and detected using a condensation particle counter. This technique allows for the detection of changes in particle morphology in response to conditioning. However, application of the technique requires a high concentration of analyte monomers prior to coagulation and may result in complex and non-intuitive signals in the mobility spectra of the output aerosol. A more detailed understanding of the dimer preparation and isolation method is necessary for the design and interpretation of experiments that use this technique. This work presents a detailed set of characterization experiments for the output of this system. The minimum monomer number concentration and minimum monomer diameter for application of this technique are presented. Physical contributions to observed mobility spectra under typical experimental configurations are identified, and conditions where dimer morphologies can unambiguously be detected and isolated are reported. Possible methodological approaches for experiments where dimer signal magnitude and/or the difference between fully uncoalesced and fully coalesced dimer mobility diameters are near noise levels are discussed, including the use of probe monomers as compensation for weak analyte monomer number concentration, potential modifications to instrument topology, and processing strategies for mobility spectra.

7IM.10

Direct Measurement of Dust Concentration by Shadowgraphy Method—Direct Image Particle Analysis (DIPA).

SHENG-CHIEH CHEN, Seungkoo Kang, Wing-Tak Lai, David Y. H. Pui, *Virginia Commonwealth University*

ISO dust injectors are generally applied to re-suspend standard dust particles, e.g. ISO A2, to challenge air filters used in internal combustion engines. The size distribution of the re-suspended dust particles is very important for acquiring the size fractional efficiency and loading performance of the filter. Generally, the existing size distributions provided by the powder manufacturer are directly applied or real-time aerosol instruments are used to

measure the particles. Various instruments, however, report different size distributions for the same dust sample and also they are quite different with that provided by the manufacturer. The main reasons are likely due to the particle transport loss during the sampling by the real-time instruments, especially for dust particles larger than 1 µm, as well as the different measurement principles and different sizing ranges of the instruments. In addition, the provided size distributions by the manufacturer are not ideal to represent the re-suspended dust particles because those distributions are measured in liquid when they are highly deagglomerated by the aids of chemical agents and ultra-sonication. In this study, therefore, the in-situ and noninvasive shadowgraph technique with an image analysis technique (particle/droplet image analysis, PDIA) were applied to measure the size of the re-suspended dusts at the moment they are being generated. The experimental system consisted of an 8 Mpixel CCD camera equipped with a high magnification micro-lens, up to 28×, to allow the measurement of small particles down to 1 µm. Monodisperse PSL particles with diameters of 5, 17 to 26 µm were generated from a homebuilt generator and used to validate the sizing accuracy of the system. Besides, the standard sized dots with 1, 3.5, 10, 50 and 100 um were used to calibrate the depth of field of the system. The validated system was then applied to measure size distribution of the widely used ISO A2 fine dusts re-suspended by different dust dispersers, including the ISO light-duty and ISO heavy-duty injectors. Results showed that there was a large discrepancy between the size distributions determined by the powder manufacturer and those from ISO injectors by PDIA, indicating the ISO injectors did not deagglomerate A2 dustswell. This study first reported the reliable size distributions for A2 dusts re-suspended by ISO injectors under different operation conditions. In addition to A2 dusts, the known sizes and known concentrations PSL particles suspended in DI water were also characterized. It was found the PDIA was able to not only accurately measure particle sizes but also directly measure particle concentration. This method should be widely applied for measuring in-situ size distribution of dust particles used to challenge the filters as well as particles in liquid.

7IM.11

FTIR Method for Continuous Real Time Aerosol Characterization for In-vivo Studies. WEI TECK TAN, Subash Krishnan, Patrick Vanscheeuwijck, *Philip Morris International Research Laboratories Pte Ltd*

The conduct of in-vivo studies as recommended by test guidelines (e.g. TG413) from the Organization for Economic Cooperation and Development (OECD) requires the test atmosphere to be held as constant as practicable. This is non-trivial especially in cases whereby the test item are complex multi-phase and multi-constituent aerosols from tobacco products or e-liquids.

Classical methods for quantification of non-gaseous key constituents such as determination of the test atmosphere nicotine concentration typically involves sample trapping in an appropriate medium followed by off-line analysis. This is resource intensive and provides only cumulative averages over the period of sample collection. For a more immediate assessment, a real time aerosol characterization method has been developed to quantify key aerosol constituents using Fourier Transformed Infrared (FTIR) spectroscopy.

The setup for sample processing, analysis and extraction from the test atmosphere consists of: 1) A dilutor which dilutes the sample to the concentration within the quantification limits of the FTIR if required, 2) A transfer section with heated tubes to vaporize non-gaseous components of the constituents to be quantified, 3) a heated filter at the end of the heated tubes to remove residual non-gaseous components to avoid damage to the FTIR, 4) a Gasmet FTIR spectrometer and 5) A vacuum pump for pulling the sample from the test atmosphere to the FTIR.

The measured overall IR spectra of the aerosol obtained from the test atmosphere is deconvoluted and compared in real time against reference calibration spectra using proprietary software from Gasmet to quantify the concentration in µg/L for water, propylene glycol, glycerol, and nicotine concurrently. During continuous sampling from the test atmosphere, concentrations of the aforementioned constituents can be quantified simultaneously by the FTIR in approximately every < 6 seconds.

Comparative studies were conducted using aerosol from e-liquids and the IQOS smokeless product whereby nicotine results from the FTIR were found to be within ±20% of the results from validated off-line analysis methods using gas chromatography. It is demonstrated that this method allows for real time quantification of selected key constituents and that can be used as a tool to further characterize the test atmosphere. When used for test atmosphere monitoring, the data generated in real time from the FTIR allows for earlier detection of process deviations and timely interventions which therefore improves the stability of the test atmosphere.

7IM.12

Correlating SMPS Size Distribution to spICP-MS Size Distribution for Flame Synthesized Titanium Dioxide Nanoparticles. NATHAN REED, Sanmathi Chavalmane, Ramesh Raliya, Sungyoon Jung, Pratim Biswas, *Washington University in St. Louis*

Flame synthesized nanoparticles are an economically significant form of nanotechnology with growing potential [1]. Due to the broad application and commercial success of these particles as reinforcing agents (e.g., carbon blacks), pigments (e.g., titanium dioxide) and flowing aids (e.g., silicon dioxide), much attention has been paid to finely controlling their properties and translating these synthesis techniques to new materials and applications. A growing body of academic work elucidates efficient routes to attain shape-controlled and highly stable nanoparticles with narrow size distributions for applications including solar cells [2], catalysts, gas sensors [3], and agricultural fertilizers[4]. Because these applications rely heavily on the controlled physical properties of nanoparticles, it becomes increasingly important to accurately and reliably measure the size distribution and chemical composition of these nanoparticles during production. Single particle inductively coupled plasma- mass spectrometry (spICP-MS) is an emerging analytical technique that measures the chemical composition, number concentration, and size distribution of nanomaterials in suspensions and aerosols. This instrument's sensitivity and dynamic range allows for improved characterization of polydisperse, aggregated, and agglomerated nanomaterials [5]. In this work, we synthesized titanium dioxide nanoparticles with geometric mean diameters ranging from 20 to 100 nm, using a flame aerosol reactor (FLAR). The nanoparticle size and extent of aggregation were characterized using transmission electron microscopy and dynamic light scattering. The size distribution of the flame synthesized titanium dioxide nanoparticles was then measured using a PerkinElmer NexION 2000 spICP-MS and a TSI Scanning Mobility Particle Sizer (SMPS) for comparison. For spherical non-aggregated nanoparticles, the spICP-MS and SMPS data closely matched; however, aggregated nanoparticle sizes were overestimated with SMPS. Our results show that spICP-MS can be effectively applied to size spherical flame synthesized nanoparticles, and even aggregated nanoparticles with a known fractal prefactor. Our results show that spICP-MS is effective for characterizing flame synthesized nanoparticle size distributions and is a complementary technique to SMPS.

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7IM.13

Can Ozone Be Used as a Calibrant for Photoacoustic Spectrophotometers? AL FISCHER, Geoffrey Smith, *University of Georgia*

Photoacoustic spectroscopy (PAS) has become a popular technique for measuring absorption of light by atmospheric aerosols in both the laboratory and field. It has low detection limits, measures suspended aerosols, and is insensitive to scattering, although it often requires rigorous calibration. Typically, the PAS instrument is either (a) filled with a gas of known concentration (N) and absorption cross-section (σ) such that the absorption in the cell (α) can be calculated according $\alpha = N\sigma$ or (b) the absorption is measured independently with a technique such as cavity ringdown spectroscopy. Then, the PAS signal can be regressed upon the known absorption to determine a calibration slope that reflects the sensitivity constant of the cell and microphone. For a calibrant to be viable for PAS, it must only undergo thermal relaxation upon exposure to light and must not (for example) undergo photodissociation at the wavelength used for calibration.

Ozone has historically been used for calibrating PAS's due to its well-known UV-visible absorption spectrum and the ease with which it can be generated. However, it is well-known to photodissociate at visible and near-IR wavelengths via the $O_3 + h\nu \rightarrow O_2 + O(^3P)$ pathway. Further, Bluvshtein et al (2017) cast doubt upon the accuracy of calibrations performed with ozone, although they saw no evidence of photodissociation and provided no explanation for the discrepancy between ozone- and particle-based calibrations. Contradicting this, Davies et al (2018) validated the accuracy of ozone calibrations and showed no problems with accuracy. The work presented here is meant to add to this discussion by presenting direct evidence of photodissociation inside the PAS cell and showing a mismatch of roughly 50% between calibration slopes obtained with nitrogen dioxide or nigrosin particles and ozone. Further, the dependence of the ozone signal on oxygen concentration will be discussed with data revealing that 5% added O_2 yields a roughly 75% increase in the PAS signal for a given concentration of ozone. These results suggest that ozone calibration may be viable but only when used with caution.

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7IM.14

Particle Detection Using the Dual-vaporizer Configuration of the Soot Particle Aerosol Mass Spectrometer. ANITA AVERY, Edward Fortner, Leah Williams, Wade Robinson, Timothy Onasch, *Aerodyne Research, Inc.*

The Soot Particle-Aerosol Mass Spectrometer (SP-AMS) can operate with one of two particle vaporizers: (1) the standard AMS resistively heated tungsten vaporizer for traditional detection of non-refractory particulate matter (NR-PM), and (2) an intracavity laser vaporizer for detection of absorbing, refractory materials, including black carbon (rBC) and metal nanoparticles, and associated NR-PM. The SP-AMS can also be operated with both vaporizers simultaneously, by sequentially turning the laser vaporizer on and laser off over the course of sampling. While each vaporizer has been shown to be effective when operated separately (with respective constraints), the use of both simultaneously is complicated by the different collection efficiencies (CE) of the two vaporizers and can strongly affect the measured NR-PM signals from both rBC-containing and non-rBC-containing particles. This work describes a systematic investigation of NR-PM (rBC-containing or not) detection, including chemical ion signatures and CE, while using dual vaporizers in the SP-AMS. The results from the combined vaporizers are compared with expected signal for laboratory generated particles and with the results from the vaporizers operated separately. Differences in detection are explained based on the separate collection efficiencies of the two vaporizers and the observed interference between the two vaporizers due to excess laser energy heating the other AMS components (e.g. the ion cage).

7IM.15

Development of Caltech Scanning-mode Nano Radial Differential Mobility Analyzer System and Its Application to Nucleation Study at the CLOUD Experiment. CHANGHYUK KIM, Huajun Mai, Wilton Mui, Stavros Amanatidis, Dominik Stolzenburg, Richard Flagan, CLOUD Collaboration, *California Institute of Technology*

Size distributions of particles can be measured by classifying the particles using the electrical mobility and detecting the number concentration of the classified particles using a condensation particle counter (CPC). However, low charging efficiency and high diffusion loss make it challenging to apply this method for particles smaller than 10 nm. Moreover, diffusion broadening reduces the resolution of electrical mobility methods when particles are classified at low voltages. For this reason, previous efforts have employed high sheath flow rates to achieve high resolution, but this has required impractically high flow rates.

The Caltech nano radial differential mobility analyzer (nRDMA) was designed to enable for classifying particles as small as 1 nm in diameter, the size range of fresh nuclei, with high resolution and compact size, but maintaining the sheath flow rates similar to those used in common DMAs. This instrument enables scanning-mode measurements of the size distribution of sub-10 nm particles with a time resolution of 2 minutes by combining the nRDMA with a non-diffusion resolving power of 10 (1.2 and 12 L/min for the aerosol and sheath flow rates, respectively) with a custom-made two-stage condensation particle counter detector. The two-stage detector was designed to grow the size of sub-10 nm particles over 100 nm by condensing diethylene glycol, and then detect them by a commercial TSI butanol CPC (3760A, d50 = 10 nm). A new, low particle-loss soft-x-ray charge conditioner was also developed to produce a well-constrained, steady-state charge distribution on the sub-10 nm particles.

This nRDMA system has been deployed in studies of the nucleation and growth kinetics of particles in the CLOUD (Cosmics Leaving Outdoor Droplets) Experiment at CERN. The relatively high resolution enables quantitative analysis of early-stage growth rates (GRs) from the measured size distribution of incipient particles formed in the CLOUD chamber. The growth rate has been calculated from the 50% appearance time at each size channel. The calculated growth rates agree well with those obtained by other aerosol instruments of the CLOUD collaboration, which proved the reliability of this nRDMA system.

7IM.16

Rational Design a Dilution Sampler for Probing Nanoparticles in Flames. ZUWEI XU, Jianlong Wan, Zhijing Su, Haibo Zhao, *Huazhong University of Science and Technology*

Dilution sampling technology is used in many process diagnostic occasions from emission monitoring to nanoparticle manufacturing (Goudeli *et al*. 2016; Zhao *et al*. 2003). This study focuses on developing a dilution sampler for online diagnostics of flame synthesis processes, with a quantitative understanding of the probe effects and reducing the perturbations on flames. Computational fluid dynamics (CFD) simulations are used to study the effects of probe geometry and working conditions on the probe performance, and ultimately to help rationalize the design of the sampling probe. It is mainly considered that changing the pressure drop, nozzle angle, sample gas temperature, and nozzle thermal conductivity affects the dilution ratio. Firstly, an optimal geometry with 30° nozzle angle is in favor of expanding the ranges of operation pressure drop and dilution ratio. The effect of flame preheating diluent gas on the dilution ratio is investigated. It can be weakened or even ignored through reducing the heat conductivity of the nozzle. When the heat conductivity is less than 1 W/(m•K), the error of the dilution ratio derived from the non-preheating assumption is estimated no more than 2%. As thus, flint glass is screened as nozzle material with the heat conductivity of 0.8 W/(m•K). For the probe of optimized nozzle angle and heat conductivity, the dilution ratio can be quantified by two easy-to-use empirical expressions in terms of the critical pressure drop as well as the linear relation between the dilution ratio and the operation pressure drop. Subsequently, a realistic probe is fabricated according to the rational design and then calibrated through a well-established setup and procedure, as thus an appropriate range of dilution ratio (about 70 ~ 350) is obtained. Combined with a commercial rotating disk thermodiluter (RTD) and a scanning mobility particle sizer (SMPS), the online monitoring system is set up to follow the spatially-resolved PSDs of TiO_2 nanoparticles in a co-flow CH_4/O_2 diffusion flame. The PSDs measured agree well with the thermophoretic sampling results as benchmark (Xu and Zhao 2015), which demonstrates the customized dilution sampler combined with the commercial SMPS possesses excellent performance and effectiveness for monitoring detailed nanoparticle evolution and spatiotemporal distribution in aerosol flames. And more broadly, it is expected that other aerosol flames, e.g., sooting flame, spray-pyrolysis flame, can be on-line diagnosed using this sample probe they have a lot in common.

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7IM.17

Near Real-Time Measurement of Crystalline Silica Aerosol Concentration Using Raman Spectroscopy. LINA ZHENG, Pramod Kulkarni, M. Eileen Birch, Kevin Ashley, Shijun Wei, *Centers for Disease Control and Prevention, NIOSH*

Long-term inhalation of aerosol containing crystalline silica can cause silicosis. Accurate measurement of crystalline silica concentrations is of great significance for the prevention of harmful exposures in industrial workplaces. Current methods have poor detection limits compared to newly imposed exposure limits of 50 µg/m^3 in the United States. Moreover, these methods cannot satisfactorily capture short-term exposures (over few minutes) that are typical in many workplaces. Developing sensitive, near real-time, field-portable methods are desired for meaningful exposure measurements and rapid implementation of exposure controls.

We present a Raman spectroscopy based method for measurement of trace airborne concentrations of crystalline silica using various aerosol micro-concentration techniques. Three aerosol micro-concentration techniques were investigated for effective coupling of collected particulate samples with micro-Raman spectroscopy: i) direct analysis on a particulate filter after focused aerosol collection using a converging nozzle, ii) analysis of dried particulate deposit on a filter obtained directly from the aerosol phase using the Spot Sampler™, and iii) analysis of a spot (∼1–3 mm diameter) obtained by redepositing the particulate sample, after low-temperature plasma ashing of an air sample collected on a filter. The deposition characteristics (i.e., spot diameter, shape, and deposit uniformity) of each technique were investigated. Calibration curves were constructed, and detection limits were estimated for α-quartz using the A_1 Raman Si-O-Si stretching – bending phonon mode at 465 cm^{-1}. The measurement sensitivity could be substantially improved by increasing the signal integration time and by reducing the particle deposition area. Detection limits in the range of 8–55 ng could be achieved by micro-concentrating the aerosol sample over a spot measuring 400–1000 µm in diameter. The low detection limits suggest that near real-time measurements of crystalline silica could be achieved with limit of quantification in the range 2–18.5 µg/m^3 at a time resolution of approximately 10 minutes at a sampling flowrate of 1.2 L/min. These detection limits were two to three orders of magnitude lower compared to those attainable using current standardized X-ray diffraction and infrared spectroscopy methods. The method was successfully extended to the measurement of α-quartz concentrations in representative workplace aerosol samples. This study demonstrates potential of portable micro-Raman spectroscopy for near-real time measurement of trace crystalline silica in air.

7IM.18

Analysis of Crystalline Silica Aerosol Using Quantum Cascade Laser-based Infrared Spectroscopy. SHIJUN WEI, Pramod Kulkarni, Lina Zheng, Kevin Ashley, *Centers for Disease Control and Prevention, NIOSH*

The objective of this study was to extend the application of a previously developed approach [1] involving quantum cascade laser based infrared spectroscopy (QCL-IR), to quantify airborne concentration of crystalline silica in workplace aerosols. This method involved collection of crystalline silica-containing aerosol on a mixed cellulose ester filter, followed by filter pretreatment using a low-temperature plasma asher to remove the organic components in the sample matrix. The ashed sample was then resuspended in aqueous phase, which was subsequently redeposited as a dried spot (1-3 mm diameter) on a polycarbonate (PC) filter. The dried spot was analyzed using QCL-IR to obtain IR transmission spectra [1]. A syringe filtration method, involving PC filter sandwiched by two orifice plates, was developed to allow redeposition of the ashed suspension as a small, dried deposit. The method was calibrated using aqueous suspensions of the α-quartz standard reference material (SRM 1878a). QCL-IR transmittance spectra in the range 750 -1030 cm^{-1}(α-quartz characteristic peak at 798 cm^{-1}) were measured and analyzed for silica content, following the approach outlined by Wei et al. [1]. A calibration model was constructed using partial least square regression to predict α-quartz mass from the QCL-IR spectra. The detection limit for α-quartz was determined to be 0.39 µg, 0.53 µg, and 1.94 µg for spot diameters of 1 mm, 1.5 mm, and 3 mm respectively. These detection limits are significantly lower than those from the current standardized X-ray diffraction (XRD) or infrared spectrometry(IR) methods. The method was extended to measurement of α-quartz concentration in workplace aerosol generated during power cutting of fiber cement and natural stone objects, and those from a coal mine dust. The measurements were compared with those from the standard XRD and FTIR methods and showed good agreement, even for samples with matrix effects and interference from kaolinite mineral. The results offer promise for further development of sensitive filter-based laboratory methods using QCL-IR spectroscopy.

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7IM.19

Characterization of Polarity Distribution of Organic Aerosol via HPLC Coupled with Fast Aerosol Size Distribution Measurements. Vikram Pratap, Yuanyuan Zhang, SHUNSUKE NAKAO, *Clarkson University*

Polarity is one of the key parameters that determine hygroscopicity of organic aerosol (OA). The polarity of OA continuously evolves as OA undergoes oxidative processing. However, direct measurements of OA polarity are limited. This study aims to determine the volume fraction of organic materials with respect to polarity by coupling a reversed-phase high-performance liquid chromatograph (HPLC) and a fast mobility particle sizer (FMPS). The column effluent is aerosolized, dried, and introduced into the FMPS. Since atomization efficiency changes as a result of the mobile-phase gradient, a second binary pump operating at an opposite gradient is introduced to maintain a constant mobile-phase composition entering the atomizer. Results show that aerosol volume concentration determined by the FMPS is linearly proportional to the mass of sample introduced into the HPLC, confirming that aerosol detection can be used as a universal detection of analytes independent of chromophores. Unlike commercial universal detection techniques such as charged aerosol detection (CAD) that provides a proxy of solute volume, the new approach allows determination of aerosol size distribution, which has a potential to provide additional information of analyte properties. This study explores the feasibility of coupling the fast size distribution measurements with cloud condensation nuclei (CCN) measurement in order to determine polarity – hygroscopicity two-dimensional distributions of organic aerosol.

7IM.20

A Gas-Inlet Design for Aircraft Sampling. DA YANG, Suresh Dhaniyala, Meilu He, *Clarkson University*

Particle rejection inlets are critical for accurate sampling of gas-phase compounds from aircraft. Traditionally, a rear-facing inlet design has been used for gas-phase sampling from aircraft. Rear-facing inlets, however, sample largely from the boundary layer of the external structure of the inlet and, thus, their measurements are likely to be compromised by the interaction of the sample gas with the cold walls of the inlet. As an alternative, we investigate the use of a side-facing inlet for gas-phase sampling. These inlets can minimize wall contact of the sampled gas, while also minimizing the largest size of the particles that will be brought in along with the gas sample. We use computational fluid dynamics (CFD) modeling along with wind-tunnel testing to investigate the relation between the large particle size sampled, wall-loss of reactive gas species, and operating conditions. The simulations will be used to identify optimal operating conditions relevant for sampling from NCAR aircraft (GV and C-130). In our presentation, we will detail the inlet design process and describe the approach to calculate gas-phase loss and particle sampling efficiencies and identify the ideal inlet operating conditions.

7IM.21

Roadmap For Statistical Calibration Model Development and Maintenance: Prediction of Organic and Elemental Carbon Composition in PM2.5 with Infrared Spectroscopy. SATOSHI TAKAHAMA, Matteo Reggente, Adele Kuzmiakova, Ann Dillner, Andrew Weakley, Bruno Debus, *EPFL*

Machine learning algorithms are becoming increasingly important for calibration of instruments (or suite of instruments) that require mathematical separation of analyte signals from analytical or electronic interferences. When physically-based models are not available for signal interpretation, data-driven models can learn discriminating features from a training set of samples to make quantitative predictions in new observations.

We summarize procedures for data preprocessing, data selection, model training, and model evaluation to determine a suitable calibration model among a suite of candidate models that can be generated. The final calibration model can include several models combined together with a classification algorithm (i.e., multilevel modeling framework) when a single model is not suitable for all sample types.

We further discuss methods for identifying limitations in model applicability. Model understanding in the form of variable importance assessment can identify the most discriminating features and how their relationships are used by the calibration model. In the operation phase of the model when reference (and possible other auxiliary measurements) are not available, methods for anticipating precision errors and large prediction errors due to biases that arise from differences in sample composition must be estimated from the primary measurement to monitor model performance. These topics are presented alongside strategies for model updating.

This life cycle of a statistical calibration model is demonstrated for calibration of thermal optical reflectance organic and elemental carbon using collocated Fourier Transform Infrared (FT-IR) spectra from several sites in the IMPROVE and Chemical Speciation Networks. This work presents a synthesis of the recent published efforts to extend FT-IR in this domain of analysis (Dillner et al. 2015a, Dillner et al. 2015b, Kuzmiakova et al. 2016, Reggente et al. 2016, Takahama et al. 2016, Weakley et al. 2016), and also includes new results.

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7IM.22

Diffusion Chargers for the Measurement of Particle Number Concentration according to the European Regulation.

Barouch Giechaskiel, YANNIS DROSSINOS, *European Commission, Joint Research Centre*

The European emissions regulation requires, the measurement of Solid Particle Number (SPN) >23 nm for type approval of diesel light-duty vehicles since 2011 (Euro 5b), for Gasoline Direct Injection (GDI) light-duty vehicles since 2014 (Euro 6) (limit $6x10^{11}$ p/km) and for heavy-duty engines since 2013 (Euro VI). Based on the Particle Measurement Program (PMP) study a minimum diameter of 23 nm size was selected to ensure the inclusion of the smallest soot particles and to exclude volatile nucleation-mode particles. Volatile particles were excluded to improve the repeatability and reproducibility of the method to levels acceptable for legislative purposes.

Real Driving Emissions (RDE) testing on the road with Portable Emissions Measurement Systems (PEMS) for SPN during type approval and in-service conformity (on-road) testing was recently (in 2017) introduced for light-duty vehicles. Furthermore, it is under discussion for heavy duty vehicles.

To date, there are two measurement methodologies available to measure SPN emissions with PEMS: (i) diffusion charging (DC) and (ii) condensation particle counting (CPC). The second methodology is applied in the regulated PMP systems. Both methodologies measure SPN emissions after thermal pre-treatment of the exhaust.

Counting efficiency curves of PMP systems and SPN-PEMS based on DCs have been recently compared (Giechaskiel et al. 2015, Giechaskiel, 2018). The relatively small size dependence of DCs is achieved with advanced systems (e.g., estimate of mean particle size and correction of results).

A comparison of the SPN-PEMS and PMP systems for various engine technologies at JRC for both light-duty, heavy-duty and L-category (mopeds and motorcycles) gave differences of the order of ±50% (Giechaskiel et al. 2015, 2016). Higher differences were observed when small particles were present, or when the concentrations were at the detection limit of the instrument, $1x10^{11}$ p/km.

The results are in good agreement with theoretically estimated differences based on the response of the instruments (Giechaskiel et al. 2014).

The authors would like to acknowledge the technical staff for their assistance in the laboratory.

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7IM.23

Comparison between ACSM and AMS at an Urban Site in Atlanta, GA: The Use of Capture Vaporizer and PM2.5 Inlet.

TAEKYU JOO, Weiqi Xu, Masayuki Takeuchi, Gamze Eris, Yunle Chen, Dao Huang, Gabriela Saavedra, Seongshik Kim, Dong Gao, Rodney J. Weber, Yele Sun, Philip Croteau, John Jayne, Nga Lee Ng, *Georgia Institute of Technology*

Aerosol Mass Spectrometer (AMS) and Aerosol Chemical Speciation Monitor (ACSM) are widely used to quantify non-refractory aerosol composition. Standard vaporizers (SV) with PM_1 aerodynamic lenses are installed in most of current AMS or ACSM instruments. While particles can bounce off from SV and decrease particle collection efficiency (CE), the new capture vaporizer (CV) has been developed and typically shows a CE of ~1 in ambient measurements. Compared to SV, CV also maintains a high CE for larger particles, which makes it possible to measure up to the $PM_{2.5}$ size range. To investigate differences in aerosol composition between the 1μm and 2.5μm size fractions in the atmosphere, a PM_1 SV-AMS and a $PM_{2.5}$ CV-ACSM were deployed at the Jefferson Street site in Atlanta, which is an urban site in the Southeastern Aerosol Characterization (SEARCH) network. Two measurement campaigns were conducted, one in summer 2017 and one in winter 2018. Aerosol volume concentration data estimated from AMS, ACSM and SUNSET OC/EC Analyzer was compared to the data from a Scanning Mobility Particle Sizer (SMPS). Positive matrix factorization (PMF) analyses were performed on ACSM and AMS data and results were compared. The differences between SV-AMS and CV-ACSM were also characterized through photo-oxidation experiments of α-pinene and β-pinene in the Georgia Tech Environmental Chamber (GTEC) facility. Organic fragmentation patterns of SV-AMS and CV-ACSM were identified from the chamber experiments.

7IM.24

Method for Chemical Analysis of Nano-Aerosol Particles – Gas-to-Particle Transitions of Highly Oxygenated Organic Molecules. ANDREA C. WAGNER, Andreas Kürten, Martin Heinritzi, Mario Simon, Joachim Curtius, *Goethe University Frankfurt*

Atmospheric aerosols are key players for cloud formation and properties. They influence our weather and climate. A large fraction of global cloud condensation nuclei (CCN) originates from nucleation. It is therefore desirable to understand the processes and substances involved in atmospheric new particle formation.

The Cosmics Leaving OUtdoor Droplets (CLOUD) experiment at CERN investigates the formation and growth of aerosol particles in an ultraclean stainless steel chamber under well-controlled conditions. Experiments simulating an urban environment were conducted. Naphthalene, trimethylbenzene and toluene were introduced as examples of anthropogenically emitted volatile organic compounds (VOCs). The oxidation of these compounds, also under the influence of nitrogen oxides, ammonia and UV light, produces highly oxygenated organic molecules (HOMs). Some of these form new particles or partition into the particle phase.

To understand the process of new particle formation, the condensing vapors need to be speciated in both gas and particle phase. For gas phase measurements of the HOMS, we are using an chemical ionization atmospheric pressure interface long time-of-flight mass spectrometer (CI-APi-LTOF) with nitrate primary ions. The measurement of the small particles resulting from nucleation is experimentally very challenging and to date, only a few instruments are capable of such an analysis. We developed a new instrument for the size-selected chemical analysis of aerosol particles from 5 to 40 nm with a lower detection limit of 10pg. The Thermal Desorption Differential Mobility Analyzer (TD-DMA) uses a semi-online principle by collecting particles on a filament and evaporating them in front of the ion reaction zone of the CI-APi-LTOF mass spectrometer. Like this, it is possible to measure both particle and gas phase HOMs with the same mass spectrometer which allows us to observe the gas-to-particle conversion or to identify species which can only be detected in one of the phases.

The particles are charged before entering the DMA-unit, which allows selecting a defined particle size. The selected particles are then collected on a filament inside the central electrode of the DMA using electrostatic precipitation. Once enough material is collected, the filament is moved outside the DMA and in front of the mass spectrometer, where it is slowly heated by an electric current. The material evaporates into ultrapure nitrogen and is detected by the mass spectrometer. Like this, the aerosol particles are separated from the gas phase to make sure only the particulate matter is analyzed and the concentration is enhanced to fit the detection limit of the CI-APi-LTOF. The LTOF by TOFWERK reaches a mass resolving power of more than 10 000 Th/Th, allowing the separation and identification of many different substances even in the complex spectra of anthropogenic HOMs.

Here, we present the instrument system of the TD-DMA regarding its setup, measurement procedures and characterization. Results comparing gas and particle phase measurements of HOMs from anthropogenically emitted precursor VOCs at the CLOUD experiment are discussed.

7IM.25

Development of a Laser-Induced Breakdown Spectroscopy (LIBS) System with Timed Ablation for a Single Particle Detection at a Low Concentration. HYUNOK MAENG, Hoseung Chae, Heesung Lee, Gibaek Kim, Haebum Lee, Kyoungtae Kim, Jihyun Kwak, Gangnam Cho, Kihong Park, *Gwangju Institute of Science and Technololgy*

The atmospheric aerosols are of current interest because of their effects on visibility impairment, human health and climate change. Especially, the chemical components of aerosols are essential to find their formation mechanisms. The elemental composition of aerosols has been commonly analyzed using filter based methods such as inductively coupled plasma-mass spectrometry (ICP-MS) and atomic absorption spectroscopy (AAS). Although these are well established techniques, they typically require a long sampling time (12-24 hours) and a series of sample pre-treatments. Also, there are not suitable for the detection of elemental variation among particles and their mixing state. In this study, the laser-induced breakdown spectroscopy (LIBS) technique was applied for the real-time detection of the elemental composition of a single particle because of its rapid detection capability. In addition, a LIBS system with timed ablation was developed by employing a continuous wave (CW) laser in front of the pulse laser to improve the low hitting efficiency (%) and hitting rate (hits/min) of single particle. This system was evaluated using laboratory-generated particles ($CaCl_2$, $MgCl_2$, NaCl and KCl) at various sizes (200-600 nm) and number concentration (50-100,000 particle/cm^3) range. Results showed the hitting efficiency (%) of 300-400 nm particles with a concentration of 50 particles/cm^3 was increased up to 80%. Also, in case of 200 nm particles, the lower detection limit (<50 particles/cm^3) was achieved compared to those obtained under the constant firing mode of pulse laser. Furthermore, the hitting rate (hits/min) sharply increased around 150 times. Lastly, results of the evaluation for the real-time detection of the mixing state of particles composed of various elements will be presented in this study.

7IM.26

Application of Laser Induced Breakdown Spectroscopy for Real Time Detection of Contamination Particles During Industrial Manufacturing. HAEBUM LEE, Hyunok Maeng, Gibaek Kim, Kyoungtae Kim, Nohhyeon Kwak, Kyungjoo Kim, Kihong Park, *Gwangju Institute of Science and Technololgy*

To assess and control possible defects in industrial manufacturing, rapid detection and identification of contamination particles are required. A stand-off laser induced breakdown spectroscopy (LIBS) system with aerosol detection chamber was developed to detect contamination particles during industrial fabrication process at high temperature and low pressure conditions. An aerosol chamber was constructed to simulate an exhaust vent pipe in semi-conductor manufacturing process at varying temperature and pressure conditions. The stand-off LIBS system detected laboratory-generated CaCl2 particles having various size (200 nm and 300 nm), and also MgCl2, NaCl, and KCl were investigated. Effects of temperature (25℃ to 250℃) and pressure (100 Torr to 760 Torr) on LIBS signal responses were further investigated. With increasing temperature, the emission line and signal-to-noise ratio (SNR) of Ca II (393.366 nm) increased and the limit of detection (LOD) was also enhanced. With reducing pressure, the emission line decreased gradually, however, it was shown that the highest SNR values were appeared at around 630 Torr. In addition, the SNR linearly decreased on the longer air mean free path (MFP). Therefore, an optimized condition of air MFP was an important factor in aerosols detection by LIBS. Although temperature and pressure affected LIBS signal responses, the stand-off LIBS system can still be useful to detect contamination particles in real.

7IM.27

Development and Field-Testing of Two Aerosol Instruments on an Unmanned Aerial Vehicle. Osku Kemppinen, Ryan Mersmann, Matthew Berg, Gavin McMeeking, TIM GORDON, *Handix Scientific*

We describe the design of two UAV-deployable aerosol instruments. The first is a mature, commercially available instrument, the Portable Optical Particle Spectrometer (POPS), from Handix Scientific LLC. The POPS is the first lower-cost instrument capable of accurately counting particles 0.15-3 micrometers in size. The POPS measures scattered light from single particles and infers particle size from scattered light intensity. The second instrument is the Holographic Aerosol Particle Imager (HAPI), which is currently in development by Kansas State University. The HAPI characterizes aerosol particle size and shape for particles larger than 5 micrometers using a novel imaging technique. In the HAPI the interference pattern between the incident and particle-scattered light is measured on a CCD sensor; this constitutes a digital hologram of a particle. The hologram is then computationally processed to render a silhouette-like image of the particle. Thus, the instrument functions as a contact-free lensless microscope, except the precise location of the particle is not required to be known, as images can be computationally focused post hoc.

Both the POPS and HAPI are lightweight and require minimal power, making them ideal for field-deployment on UAV platforms. We will present the first results of POPS flight tests, reporting how propeller wash, vibration, and other flight-related issues affect measurements compared to a reference POPS located on the ground. We will also discuss the possibility of deploying the POPS and HAPI instruments together to enable particle characterization across the sub- to super-micrometer particle size range on a single UAV.

7IM.28

Development and Evaluation of Dry Powder Aerosol Generator with Nozzle and Magnetic Stirrer for Inhalation Toxicity Testing of Nanomaterials. GUN-HO LEE, Kang-Ho Ahn, *Hanyang University, R. of Korea*

Recently, with the rapid development of nanotechnology, many nanomaterials are being produced. These nanomaterials have unique characteristics that are quite different from those in the lump form and are widely used in many industrial fields. However, these nanomaterials may enter the body through the respiratory tract and cause pulmonary fibrosis in the lungs or may precipitate in the alveoli causing inflammation, which may be transferred to other organs through the blood vessels in the lungs, leading to secondary toxicity. As a result, the current risk assessment of nanomaterials is becoming a global issue. In order to perform inhalation toxicity testing, one of the methods for evaluating the risk of nanomaterials, an aerosol generator is important. It can make aerosol which can be inhaled by laboratory animals.

In this study, we developed a dry powder aerosol generator for inhalation toxicity testing of nanomaterials. The developed dry powder aerosol generator was evaluated for the factors that could affect the aerosol generation, mock inhalation toxicity testing verified that performance of aerosol generation is satisfied with recommendations of OECD test guideline. Finally, the short-term / sub-chronic inhalation toxicity testing of CNF was performed using a dry powder aerosol generator to verify the performance of an aerosol generator for inhalation toxicity testing of nanomaterials. Finally, short-term/ sub-chronic inhalation toxicity testing of CNF was performed using a dry powder aerosol generator and the performance as an aerosol generator for inhalation toxicity testing of nanomaterials was verified. The dry powder aerosol generator developed in this study is expected to contribute to the study of inhalation toxicity study of nanomaterials.

7IM.29

Direct Sampling of Sub-µm Atmospheric Particulate Organic Matter at Sub-ng m-3 Mass Concentrations by Proton-Transfer-Reaction Mass Spectrometry. MARKUS MUELLER, Andreas Klinger, Gregor Mayramhof, Joris Leglise, Todd Rogers, Armin Wisthaler, *IONICON Analytik GmbH., Innsbruck, Austria*

The chemical characterization of the organic fraction of atmospheric particulate matter is still a challenge. Herein we present the novel modular "Chemical Analysis of Aerosol Online" (CHARON) particle inlet coupled to a new-generation proton-transfer-reaction time-of-flight mass spectrometer (PTR-TOF 6000 X2, Ionicon Analytik, Austria). The PTR-TOF 6000 X2 detects organic analytes in real-time at sub-pptV levels by chemical ionization with hydronium reagent ions. The CHARON inlet consists of a gas-phase denuder for stripping off gas-phase analytes (efficiency >99.999%), an aerodynamic lens for particle collimation, an inertial sampler for the particle-enriched flow and a thermodesorption unit for particle volatilization. With an enrichment factor of ~30 for particle diameters (DP) between 120 nm and 1000 nm (lower enrichment for particles in the 60-to-120 nm diameter range), the CHARON PTR-TOF 6000 X2 system detects particulate organic matter online and in real-time down to 200 pg m^{-3}. Proton transfer from hydronium ions quantitatively ionizes almost the full range of organic analytes in the intermediate to low volatility range. The high mass resolution (R > 6000) and mass accuracy (< 10 ppm) of the Ionicon PTR-TOF 6000 X2 allows to assign elemental compositions to organic analyte ions over a large mass range. We will present a detailed characterization of the CHARON PTR-TOF 6000 X2 instrument and first results from ambient air measurements in Innsbruck (Austria).

The development of CHARON was funded through the PIMMS ITN, which was supported by the European Commission's 7th Framework Programme under grant agreement number 287382. J.L. received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement number 690958 (MARSU).

7IM.30

Laboratory Testing of Gas Exchange Efficiency in a Cylindrical Counter Flow Denuder. HAGINO HIROYUKI, *Japan Automobile Research Institute (JARI)*

Many applications for aerosol particle measurement and calibration particle generation require removal of gaseous components. Diffusional separation techniques are widely used for this purpose. However, the use of these denuder techniques is limited when less reactive and/or inert gases (i.e., O_2, CO_2, and H_2O) need to be exchanged continuously. In this study, a cylindrical counter flow denuder was developed using a microporous glass tube to obtain a denuder system that had exchange of gases. The denuder performance for gas exchange was evaluated using experimental parameters in a laboratory test.

The denuder was designed to exchange gases in the sample flow by diffusion to the purge flow across a cylindrical microporous glass tube. The cylindrical counter flow denuder had two concentric tubes; an inner porous tube through which aerosol particles were passed as sample flow; and an outer tube made of seamless stainless steel with counter-current purge gas supply as purge flow, in opposite direction to the sample flow. The inner tube for sample gas flow was designed with maximum dimensions and had a center channel (250 mm length, 5 mm o.d., and a pore size of 0.1 µm) through which the aerosol and gas were passed. Several evaluation tests for gas exchange were performed with sample flow tubes made of different types of outer tube and the length counter-current flow diffusion denuder. The sample flow rate of the counter flow denuder was set at 0.15 L/min, as it was used as an inlet of the Aerosol mass spectrometer (AMS).

Laboratory test results indicated that removal efficiencies of gases increased with higher sample to purge flow rate ratio. However, the dimension of outer that was related with purge gas residence time did not affect significantly gas removal efficiency following optimization of sample and purge flow rate conditions. Significantly high gas exchange efficiency was obtained for the length of the denuder that is corresponding to the residence time in sample flow channel.

7IM.31

Direct Measurement of Trace Multi-Elemental Aerosols using Inductively Coupled Plasma Time-of-Flight Mass Spectrometry and X-ray Fluorescence Spectroscopy. HAGINO HIROYUKI, Martin Tanner, Olga Borovinskaya, Toshihide Hikita, Akio Shimono, Kohei Nishiguchi, Yusuke Mizuno, *Japan Automobile Research Institute (JARI)*

Inductively coupled plasma mass spectrometry (ICP-MS) is widely used when rapid and sensitive detection for a wide range of elements of airborne particles is required in many situations, such as the monitoring of the ambient particulate matter (PM), emission sources, and the clean room air for semiconductor manufacture processes. In analysis by ICP-MS, the airborne particles are usually collected on filters and elemental analysis is carried out through pre-processing on the resultant sample, as well known as off-line analysis. This off-line analysis using ICP-MS takes time for a day or a few days, and reduces the time resolution about the behaviour of particle concentration.

For on-line and real-time analysis of aerosol samples using ICP-MS, the gas exchange devices (GED) which followed by the replacement of air with argon and transported to the ICP-MS is need to be equipped due to sustaining the plasma (Nishiguchi et al., 2008). The bulk aerosol sample were produced by a GED with ICP-MS that exchanges the gas molecules from air to Ar the resulting gas-converted air sample can be introduced directly into the ICP-MS instrument. However, the ICP-MS used a quadrupole mass spectrometer (ICP-QMS), a detailed study on the signal fine structure with scanning-based mass spectrometers but no simultaneous multi-element measurement was possible. In order to further improve time resolution of the ICP-QMS and to extend its capabilities to determine single particle information, ICP-MS equipped with the Time-of-Flight Aerosol Mass Spectrometer (ICP-TOFMS) was developed recently (e.g. Martine and Günther, 2008) and provided commercially (icpTOF, Tofwerk).

This study describes a direct trace multi-elemental aerosol measurement in which an icpTOF (Aerosol-icpTOF) has been eqipped with a GED (GEDIII, J-Science Laboratory). This Aerosol-icpTOF is the real-time, field-deployable, aerosol mass spectrometer that is capable of directly distinguishing the elemental composition of ions having the same nominal mass and will be described the more details in elsewhere (Hagino et al., In-preparation).

The trace elements in ambient $PM_{2.5}$ were measured by using the Aerosol-icpTOF and the continuous particulate monitor with X-ray Fluorescence (XRF) (Model PX375, HORIBA). The icpTOF and XRF are a fundamentally different instruments. However, there were the high degree of correlation as trace element concentrations during the 1-h time resolution.

7IM.32

Control of Number Concentration of Aerosol Nanoparticles Generated by Nanospray Drying. MASAKI SAKAMOTO, Fumitaka Ichihara, Takafumi Seto, Yoshio Otani, *Kanazawa University*

Generation of test aerosol particles with a narrow size distribution and a precise number concentration is important for various aerosol experiments such as filtration test and the calibration of particle counters. In terms of uniformity of particle size, polystylene latex (PSL) microspheres have been widely used as standard particles with size range from nanometer to micron. Spray drying method is generally used to obtain the monodispersed PSL test particles in the aerosol phase. However, in the spray drying process, it is difficult to precisely control the number concentration of aerosol. Small amount of impurity contained in the PSL suspension may produce residual nanoparticles of undesirable size and it sometimes increases the number concentration of test aerosol. Reduction of atomized droplet size is known to be effective in decreasing the effect of these contaminants.

In this study, a new atomizer is designed to generate droplets with a peak diameter smaller than 200nm. In order to reduce the contamination, an ultrapure water system was connected to the atomizer. The PSL solution with a known liquid-based concentration was introduced to the atomizer by a syringe pump. The gas phase concentration was measured by a laser particle counter (LPC, >0.1micron, Met ONE model A0100B) and a condensation particle counter (CPC, >4nm, TSI model 3775). The background aerosol concentration with the introduction of ultrapure water was 0.5/cc-gas by the LPC and 1670/cc-gas by the CPC. The relationship between liquid-based PSL concentration and the aerosol concentration was analyzed by changing the diameter of standard particles (100, 200, or 500 nm) and the concentration of the PSL suspension (10^4 to 10^7 /cc-liquid). The minimum controllable aerosol concentration was as small as 0.1 particle/cc-air for the LPC and 1000 particle/cc-air for the CPC.

7IM.33

Application of Centrifugal Filter to Measurement of Aerosol Size Distribution. RYO OZAWA, Yoshio Otani, Takafumi Seto, *Kanazawa University*

In recent years, with the growing interest in indoor air quality and the atmospheric environment, removal and analysis of aerosol is becoming increasingly important. Although there are various filters suitable for the particle size range and type of aerosol, few filters can maintain a high aerosol collection efficiency while keeping a low airflow resistance. We have proposed a new type of air filter called as “centrifugal filter” in which a cylindrical filter rotates along the axis parallel to the air flow (Nakajima et al. 2015). The collection efficiency of centrifugal filter is adjustable by changing the rotation speed without changing the pressure drop. Since the collection efficiency of centrifugal filter is varied by changing the rotation speed of filter to attain various cut-off sizes, it may be combined with a particle detector which does not have size-discrimination capability to form a new type of measurement system. By scanning the rotation speed of centrifugal filter followed by the detection of total aerosol concentration, and applying an appropriate inversion scheme from the particle penetration to the size distribution, we may construct a real time aerosol measurement system based on the aerodynamic size as SMPS measures the size distribution based on mobility diameter by scanning the voltage. However, because the classification performance of the centrifugal filter is not so high, inversion method using 50% cutoff diameter cannot be used. In this work, we developed the new inversion method that gives frequencies of an arbitrary size distribution function by using a least square method. We applied the inversion method to the measurement of size distribution of Kanto Loam test dust (JIS-11). JIS-11 particles were dispersed by a fluidized-bed aerosol generator (Model 3211, Kanomax Inc.) and electrically neutralized and mixed with a clean air to make the volumetric flow rate equal to 7 L/min. The inlet and outlet concentrations of JIS-11 were measured with a photometer (Dust track, Model 8530, TSI) by changing the rotation speed of centrifugal filter. We compared the size distributions of particles converted by the present inversion method and those measured by an optical particle counter (OPS, Model 3330, TSI). As a result, we found a good agreement between those measured by the centrifugal filter and the OPS.

7IM.34

Difference in the Sampling Artifacts During Aerosol Collection between Cyclone and Filter. DAIKI SHISHIDO, Tomoaki Okuda, *Keio University*

In recent years, the influence on health by fine aerosol particles such as PM2.5 has been concerned. For this reason, it has become necessary to identify the factors (such as chemical components), that determine health effects. However, utilized filter collection of PM2.5 could occur unexpected artifacts, for example, adsorption of gaseous substances, chemical reaction with particles and volatilization of semi-volatile components. Therefore, we developed a high-volume simultaneous sampler for fine (PM2.5) and coarse aerosol particles using the impactor and cyclone techniques. This device can collect PM2.5 as powder form without the use of filter. In this study, we collected PM2.5 using the new method (virtual impactor and cyclone), and a conventional method (real impactor and filter), and analyzed these chemical components. As a result, it was found that the loss of nitrate may be caused in filter collection, however, the loss of nitrate may be prevented in cyclone collection.

7IM.35

Particle Measurement of Coal-Fired Power Plant Exhaust from the Stack Using Dilution Probe. CHANG GYU WOO, Hak-Joon Kim, Bangwoo Han, Yong-Jin Kim, Suji Kang, Sungnam Chun, *Korea Institute of Machinery and Materials*

Emissions from stationary sources such as power plant attracts much attention due to intense emission control in Korea. 26 power plants are located in Chungnam area which is important for the air quality of capital area. Current exhaust particles are monitored using opacity measurement. The measurement results are not size-resolved and small particles under several tens of nanometers cannot be measured. For the size-resolved filterable particle measurement, dilution probe technology are prepared. Continuous, real-time measurement technology for the precise fine particle ($PM_{2.5}$) monitoring is suggested in this research. Exhaust particles are sampled through dilution probe and are measured light scattering method. EPA method 201a is simultaneously adopted to compare the values. Air flowrate and temperature of dilution air controlled to find optimal measuring condition. This work was supported by the Korea Institute of Energy Technology Evaluation and Planning (KETEP) and the Ministry of Trade, Industry & Energy (MOTIE) of the Republic of Korea (No.20161110100140).

7LC.1

CitySpace Air Sensor Network: Application of High-Time Resolution Data from a Network of Low-Cost Air Sensor Technology to Examine Urban Air Pollution. STEPHEN FEINBERG, Ron Williams, Gayle Hagler, Judy Low, Larry Smith, Ryan Brown, Daniel Garver, Michael Davis, Michael Morton, Joe Schaefer, John Campbell, Tim McArthur, *ORISE/ORD-US EPA, RTP, NC*

Recent advances in air pollution sensor technology have occurred that could help address concerns about nearby sources, support the siting of regulatory monitoring stations, and increase the knowledge of spatiotemporal variation of air pollution and associated health effects. Sensors are now being developed that are much smaller and lower-cost than traditional ambient air monitoring systems, and in some instances with promising performance. Thus, these sensors have the capability of being deployed in a nodal pattern to provide greater coverage of a geographical area. One such example is the CitySpace project conducted by the US EPA and the City of Memphis Health Department. A total of 16 solar and/or land powered sensor pods were developed containing Alphasense OPC-N2 particulate sensors along with ancillary monitoring components and were deployed across Memphis, TN for six months. Six of those sensor pods were determined to meet selection criteria for further analysis based on collocated comparison with a regulatory Tapered element oscillating microbalance (TEOM) monitor. The data from these pods were then normalized to imitate TEOM measurement, and the resultant concentrations were used in an analysis to examine potential contributors to urban air particulate matter. The 1-minute data from the sensor pods were used to perform a receptor modeling technique called Nonparametric Trajectory Analysis (NTA). The NTA results from the network of sensors were used to explore which regions within the study area were associated with high measured concentrations and what potential sources are within those regions.

7LC.2

Field Performance Evaluation of Four Low-Cost Particulate Matter Sensors. ANDREA CLEMENTS, Manu Srivastava, Teri Conner, Joann Rice, Bruce Habel, Stephen Reece, Ron Williams, *U.S. EPA Office of Research and Development*

Low-cost (<$2500) particulate matter (PM) sensors are appealing to many stakeholders including professional researchers, community groups, and citizen scientists. Although the low-cost, compact size, and portability of air quality sensors makes these devices attractive for community level monitoring and for citizen science applications, detailed performance evaluations are needed to better understand the data quality. In recent years, the U.S. Environmental Protection Agency (EPA) has conducted a number of evaluations on low-cost air quality sensors with full results published on the Air Sensor Toolbox for Citizen Scientists, Researchers and Developers (www.epa.gov/air-sensor-toolbox). This work presents results from the evaluation of four PM sensors – TES 5322 Air Quality Monitor, Plantower PMS 7003, PurpleAir PA-II-SD, and Aeroqual Portable Particulate Monitor PM10/PM2.5. Each sensor was deployed in triplicate for a period of at least 30 days between October 2017 and March 2018 at the Ambient Air Innovation Research Site (AIRS) test platform on EPA’s campus in Research Triangle Park, NC. Sensors were collocated with nearby meteorological and Federal Equivalent Method (FEM) instruments, and data were compared to evaluate the sensor performance. Results include comparison to FEM measurements (accuracy, bias, reproducibility), examination of environmental variables (e.g. temperature, relative humidity) that influence performance, and observations about the ease-of-use and reliability of each sensor.

Although this abstract was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

7LC.3

Deposition Characteristics of Bioaerosols: Towards Black Silicon-Based MEMS Bioaerosol Detection. UGUR SOYSAL, Evelyne Géhin, Frédéric Marty, Emmanuelle Algré, Charles Motzkus, *Université Paris-Est, CERTES*

As excessive exposure to bioaerosols results in adverse health effects, the development of real-time bioaerosol detection is highly relevant. Widely used systems are bulky, time-consuming or expensive to maintain. Over the past decade, sensor developments have shown the following features: portable, inexpensive, and suitable for monitoring real-time measurements. With respect to the semiconductor industry, airborne particle monitoring systems can be easily accessed through the development of silicon-based nano/micro scale systems and can be achieved by combining an appropriate sampling method with miniature sensors. Nano and micro electromechanical (NEMS/MEMS) sensors could be promising tools for bioaerosol detection, and provide real-time mass concentration measurements, particularly in terms of sensitivity. However, reducing the size of the fundamental aspects of aerosol sampling methods reveals strengths and limitations in the systems. Unlike typically used sampling methods in the case of traditional particle detectors, the collection efficiency cannot be the only concern to characterize the utility of nano/micro scale detection systems. Due to the arbitrarily shaped and sized NEMS/MEMS sensors, the deposition characteristics such as deposition shape and size should be investigated and adapted to the developed sensors in order to obtain a high sampling efficiency.

In this work, we have designed and fabricated a multiple round nozzle single-stage bio-impactor based on classical impactor design theory. While the design value of cut-off diameter is 0.4 µm, the operating flow rate and Reynolds number are 10 LPM and 2825, respectively. To study the deposition characteristics of bioaerosols, we have generated monodispersed particles with various sizes (aerodynamic median diameter: 0.91 µm ± 0.01 µm, 2.07 µm ± 0.01 µm, 2.5 µm ± 0.03 µm and 3.8 µm ± 0.004 µm) of fluorescence particles as test particles, Aspergillus niger spores, Staphylococcus epidermidis, and Pseudomonas fluorescens with aerodynamic median diameters of 3.00 µm ± 0.01 µm, 0.73 µm ± 0.01, and 0.66 µm ± 0.007 µm, respectively. These particles have been impacted on silicon and nanostructured silicon (i.e. black silicon, pillars a few nm dia and ~ 3.00 µm length) surfaces as an impaction plate of the designed impactor. Although the properties of the biological and non-biological test particles used in this study are different, their deposition characteristics show similarities and the deposition patterns correlated with the size of each type of particles.

Preliminary results show that the halo-shaped, ring-shaped or only primary deposit (underneath the nozzle) have been observed for silicon and black silicon impaction plates. A halo type pattern consists of a primary deposit in the center that is surrounded by a secondary deposit. A ring-shaped pattern forms a particle-free area underneath the nozzles, thus the deposit encloses this area. There have been only a few study discussing the reason for the deposit shapes and those are contradictory. Herein, we show that the halo and ring-shaped deposits occur due to rebound or re-entrainment of the particles on a flat silicon surface. As the particle diameter is increased from sub-µm to micron size, the deposits have changed from the halo to ring shape. All the sub-µm size particles have demonstrated a similar halo type pattern in turn an enlarged deposition area. Although black silicon has not significantly affected the deposition characteristics of sub-µm particles, it breaks all the micron size particles into fragments and provides a localized circular deposition pattern (dia < 500µm) underneath the nozzle which is smaller than the nozzle diameter (500 µm). The sharp nano pillars have enabled to reduce bouncing effect, thus have provided a confined deposition pattern, which can be easily aligned with the micro sensor. Though porous substrates are often avoided in impactors due to the penetration of the impinging jet that causes excess particle collection, which leads non-ideal collection efficiency curves, it can be negligible for large cut-off diameters as in this work. Therefore, we propose that black silicon implemented MEMS mass sensors are favorable for the detection of micron size particles like Aspergillus niger spores.

7LC.4

Portable Digital Holography Instrument for In-situ Coarse-mode Aerosol Imaging. OSKU KEMPPINEN, Matthew Berg, Yuli W. Heinson, Stephen Holler, *Kansas State University*

Digital holography is a contact-free imaging method that doesn't require trapping or otherwise preparing the imaged particle prior to the measurement. We have designed and are currently manufacturing a proof-of-concept model for a lightweight, low-cost digital holography instrument that can image freely flowing particles, sizes ranging from tens of micrometers up to millimeters, in the atmosphere. We have also developed the necessary algorithms to automatically reconstruct the particles’ two-dimensional silhouettes, with additional limited three-dimensional information. It is expected that the final product will have capabilities to run these algorithms on-board the instrument, giving the instrument near-real-time analysis capabilities.

The current estimate for the mass of the instrument is approximately 5kg with batteries, light enough to be flown on an off-the-shelf Unmanned Aerial System (drone), with approximately 20-30 minutes of flight and measurement time between landings. The current material cost estimate for the prototype model is roughly $7000, but it's expected this can be reduced for future models.

The instrument concept, if proven successful in the upcoming test campaign, will allow imaging large atmospheric particles almost anywhere in the lower boundary layer with minimal set-up required, and with very low operational costs. We expect the instrument will greatly add to the knowledge of coarse-mode aerosol particle morphology by providing statistically significant amount of measurements that have been slow, costly, and in some cases impossible to perform thus far.

7LC.5

EPA’s Village Green Sensor-Based Air Monitoring Stations: Long-term Performance of PM2.5 Sensors. TERI CONNER, Sue Kimbrough, Ron Williams, Brad Johns, John White, Gayle Hagler, *US EPA - ORD, RTP, NC*

The Village Green Project was established to demonstrate the capabilities of new real-time monitoring technology and to help communities learn about local air quality by locating EPA-developed sensor-based air monitoring stations in publicly accessible locations. A pilot station in Durham, North Carolina demonstrated the system’s ability to monitor several common air pollutants in real-time and make the data available online. The Village Green Project has since expanded to seven additional locations across the U.S. to evaluate the station’s operation under different weather conditions and to increase awareness of this new community-based air quality monitoring system. The solar and wind powered station is a park bench structure with instruments that provide minute-to-minute air measurements for ozone, particle pollution and weather conditions. Though the overall goal of the project is to provide the public and communities with information previously not available about their local air quality and engage communities in air pollution awareness, the data acquired at these stations provide EPA researchers with the opportunity to evaluate long-term performance of sensor devices. Some stations have been reporting PM2.5 data approaching 2 years. In this presentation, we report on the long-term performance of the Village Green station PM2.5 sensors (MIE pDR-1500, Thermo Scientific) deployed in a variety of locations and conditions.

7LC.6

Evaluation of a Multi-wavelength Black Carbon Sensor. AMARA HOLDER, Brannon Seay, Sue Kimbrough, Johanna Aurell, Steven Blair, Jeff Blair, *U.S. EPA*

Black carbon emitted from incomplete combustion processes is often used as a marker for diesel exhaust, a known carcinogen, and is associated with adverse health effects in exposed communities. Although multiple instruments exist to measure black carbon, very few are tailored for sensor applications where light-weight, low-power, and insensitivity to environmental conditions allow for operation in the demanding environments encountered during unmanned aerial measurements or long-term fence line monitoring as conducted by the US EPA. Understanding these challenges, Aethlabs (San Francisco, CA) designed the MA200/MA350 multi-wavelength black carbon instruments. We assessed the operation of these new sensors compared to numerous other black carbon instruments under a variety of ambient environmental conditions and black carbon concentrations. In long-term ambient measurements the new sensor compared well with heavier, multi-wavelength, rack mounted instruments and were only minimally impacted from changing ambient conditions. The sensor was also affixed to a tethered aerostat and an unmanned aerial vehicle for sampling from open biomass burning. Compared to another commercially available light-weight black carbon instrument, the new sensor was able to sample for longer times in the high concentration plume due to an automatically advancing, multi-spot filter tape. Additionally, the new sensor employed a self-correction for artifacts due to filter loading, increasing the accuracy of the black carbon measurement.

The views expressed in this abstract are those of the authors and do not necessarily reflect the views or policies of the U.S. Environmental Protection Agency.

7LC.7

A Device Development for Measuring Atmospheric Columnar Integrated Air Pollution. Hardik Gajjar, DAYA KAUL, *Pandit Deendayal Petroleum University*

Aerosols have varied impact on climate and human health. Aerosols of highly scattering in nature increases the albedo of the earth and thereby cools the surface and thus, effectively offsets greenhouse gas warming by about 25-50%; whereas, absorbing types of aerosols (e.g. black carbon) absorbs solar radiation, hence increases the surface temperature; Absorbing types of aerosols are largely present in urban environment due to presence of relatively larger number of vehicle fleet and subsequent more fossil fuel combustions than in rural areas. This aggravates the already present Urban Heat Island (UHI) induced atmospheric heating due to almost ubiquitous presence of concrete structures in urban areas.

One of the important parameters in aerosol measurement is aerosol optical depth (AOD). Several instruments and techniques are used to measure AOD such as with satellite and ground based sun-photometry, ground and airborne radiometers and LIDARs. The ground based sun photometry is preferred more over other approaches because of its customizable spatial and temporal resolution and good accuracy. Satellite data is also most frequently used due to its large spatial coverage; however its accuracy is always under much debate due to improper treatment of reflection and aerosol models used in AOD algorithm. The uncertainty is even more significant over areas where satellite overpass does not coincide with the area or period of interest and nearest satellite pass data is approximated and is considered for studies. The airborne radiometer and LIDAR retrieval are able to derive vertical profile of AOD and have flexible measurement recording time. Still these are not in widespread use for AOD monitoring because they require complex instrumentation and high maintenance cost is always an issue for areas where technical and financial support are acutely limited.

In response to bring down the cost, affordability and portability problem, a camera based AOD retrieval was developed which measured AOD at three wavelength using CMOS sensor of camera. Certain modifications were required to do so, which included addition of narrow band pass and neutral density filters to protect the image sensor and not to allow saturation of solar images produced. The details of the method, instrument and result will be presented in the conference.

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7LC.8

Smart Air Quality Network, the Measurement Network for the Future. VOLKER ZIEGLER, Markus Pesch, Matthias Budde, Michael Beigl, Till Riedel, Johannes Riesterer, Klaus Schäfer, Stefan Emeis, Duick Young, Josef Cyrys, Juergen Schnelle-Kreis, Andreas Philipp, Erik Petersen, Johanna Redelstein, Hans Grimm, Stefan Hinterreiter, Thomas Gratza, *GRIMM Aerosol Technik Ainring GmbH & CO.KG, Germany*

Air Quality and with this, subjective and health related life quality, is one of the biggest topics of modern cities and developing countries in our time. For many regions and cities it is difficult to take action regarding air quality in mobility, residential or working areas, because there is no fine-meshed and profound database available for making right decisions in time.

Although the required basic data as well as the measurement principles would be available, a proper platform for connection, combination and evaluation of measurement data to get profound decisions is still missing. SmartAirQualityNetwork shall be a very pragmatic and data driven attempt in which all available data will be combined with mobile measurements to an integrated measurement strategy for the first time.

With the connection and combination of open data sources, such as meteorological data, research data about air pollution levels, city development plans, remote sensing data about influencing factors as mixing layer heights, comprehensive coverage with ultra-low-cost-Sensors, “scientific scouts”, demand-oriented usage of UAVs together with methods of real-time-modelling and analyzing, a new measurement and analyzing concept will be developed. In the test region of Augsburg (Bavaria, Germany), the intension is, to establish a prototype of a measurement network 2.0 using IoT-Methods and analytics of big data that will be able to be scaled and multiplied to any other region. The main target is to give new real time information that can be used for several in-time actions based on air pollution levels such as alternative routing in navigation systems.

High polluted zones and traffic control activities in order to reduce traffic and pollution levels as well as to inform people via mobile apps about pollution levels will be given and recommendations for actions and valuable information for clean air strategies will be developed. Beside a broad awareness of possible influencing factors to the public as well as for decision makers, it will provide a broad database for controlling an increased individual mobility, alternative mobility concepts and development of new traffic control systems.

Funding: Federal Ministry of Transportation and Data Integration of the Federal Republik of Germany (mFund)

7LC.9

Application of Consumer-grade Sensors to Study the Effect of Heatwaves on Indoor Air Quality. RUIKANG HE, Gediminas Mainelis, Ioanna Tsoulou, Sanjeevi Thirumurugesan, Brian Morgan, Stephania Gonzalez, Deborah Plotnik, Jennifer Senick, Clinton J. Andrews, *Rutgers, The State University of New Jersey*

Global climate change is affecting extreme weather, including the duration, frequency and intensity of heatwaves (e.g., extended periods of hot temperatures). We hypothesized that low-income seniors who live in urban areas are affected the most by the heatwaves because they often are physically frail and may have limited access to air conditioning. We recruited 24 seniors in three different buildings (sites M, F, and L) in Elizabeth, NJ, to participate in a study from July to September during which we deployed consumer-grade sensors in individual apartments to monitor indoor and outdoor air pollution levels, air temperature, relative humidity, CO_2, and strategies to cope with heat (e.g., air conditioner use, window operation, and use of communal spaces.) The selected study city has some of the worst air pollution in the state due to its proximity to oil refineries, Newark airport, NJ Turnpike, and the Port of Newark and New York.

In preparation for the study, we developed and deployed sensor networks in each apartment. AirVisual Node (Air Visual Ltd.) measured PM2.5 as well as temperature and relative humidity; a reference unit was installed outdoors. AirVisual was selected for this study based on our comparison of this tool with other consumer-grade sensors. Wemo Insight (Belkin International) monitored energy consumed by the appliances and provided window air-conditioner usage information. Window Open/Close Sensors (Monnit) told us when the windows were open/closed. All data were transmitted via local WiFi hubs.

Our findings show that air pollution levels indoors were affected not only by outdoor pollutant levels and outdoor temperatures but also by building conditions and individual behaviors of seniors, including smoking in the apartments, their ability to use of Air Conditioning (A/C) due to cost concerns and relocation to outdoor shaded areas or air-conditioned common areas within their buildings during hot days. The average PM2.5 levels and Indoor/Outdoor PM2.5 (I/O) ratios were 84.78 $\mu g/m^3$ and 14.96 in smokers' units, and the same parameters were 14.86 $\mu g/m^3$ and 2.30 in non-smokers' units. The non-smokers' apartments without A/C (site M) had the average I/O ~1.3 for both heat wave and non-heatwave days, while the apartments with A/C (sites F and L) showed I/O decrease from ~2.1 during non-heatwave days to ~1.1 during heatwave days. Interestingly, the I/O ratios became more strongly correlated with outdoor temperature during the heatwave days and had overall lower I/O values compared to non-heatwave days (sites F and L). For CO_2, the concentration across apartments varied between 500 and 2000 ppm, with multiple readings above 1500 ppm after 7 pm, which was highly affected by individual behaviors of the residents.

In summary, our findings demonstrate the utility and usability of consumer-grade air quality sensors to study factors affecting indoor air pollution. Our data also suggest that long-term adaptation and resilience to climate change could benefit from an integrated resident-to-building-to-neighborhood evaluation. This research was funded by NSF grant AGS-1645786.

7LC.10

In-Situ Spectroscopic Analysis of PM Chemical Composition in a Low-Cost Particle Collector. HE JIAYANG, Byron Ockerman, Igor Novosselov, *University of Washington*

The toxic potential of inhaled particulate matters (PM) is dependent on particle size, number density, and their chemical composition. Within the respiratory tract, particle size determines the region of deposition, residence time, solubility and tissue uptake; the particle's chemical composition determines the potential for biochemical reaction with tissue and cells. Identifying the sources of fine and ultrafine PM exposure is necessary for effective health-related interventions for sensitive population (i.e., asthma patients). Currently, epidemiological studies rely on filters or inertial impactors to sample particulates, those often have problems with ease of use and substrate overloading. The ability to collect particles in a wide size range is essential for personal samplers enabling a comprehensive assessment of the PM exposure. However, it is challenging to collect particles over a wide size range with high collection efficiencies within one sampler due to the mismatch in particles electrical mobility and their inertial properties. We present the design and evaluation of a compact, low-cost cartridge that uses inertial and electrostatic collection mechanisms. The low weight of the cartridge (< 1.5 g) allows for gravimetric sample analysis. The compatibility with pipette elution allows for simple sample elution procedure. The collection performance of the cartridge was evaluated in laboratory studies using polydisperse ceramic particles and combustion-generated aerosols. Typical collection efficiencies are above 80% for inert particles and above 60% for combustion-generated PM. The cartridge is fabricated using UV transparent material, enabling in-situ fluorescence analysis of the collected sample. Compatible with standard cuvette holders, the cartridge can be analyzed using standard laboratory equipment.

7LC.11

A Study Using Open-face Passive Samplers to Measure PM Concentration. ZHONG-MIN WANG, Yixin Zhou, Fraser Gaspar, Bradman Asa, Ryuzaburo Kamiya, *California Department of Public Health*

Simpler and less expensive samplers for monitoring exposures to airborne particulate matter (PM) in indoor environments are needed. In 15 northern California childcare facilities, we deployed open-faced poly-carbonate substrate passive aerosol samplers (OPS) and then used computer controlled scanning electron microscopy to measure indoor PM particle size, number, and elemental concentration. Particle concentration were compared to PM concentrations measured by filter-based active samplers. The Pearson's correlation coefficient between PM mass concentrations estimated from the OPS versus gravimetric methods was 0.77 for PM2.5 and 0.95 for PM10, respectively, indicating positive correlation between the passive and active sampler results. PM and elemental composition varied by facility location and interior characteristics of the childcare facilities such as floor type, presence of combustion source, occupant density, and the level of activity. The rich carbon content in the polymer-based polycarbonate substrate produced positive bias in the carbon concentration analysis. Based on the carbon concentration determined using a copper substrate, a correction factor was needed to determine the total carbon concentrations in the sampled PM for the polycarbonate substrate passive sampler. Overall, the results demonstrated that the OPS collected sufficient aerosol particles in one business day (6-8 hours) to assess PM levels.

7LC.12

An Electric Impaction Sensor for Detecting PM2.5. CHEN TZU-MING, Hsu Jung-Nan, Fan-Lun Chen, Shuenn-Chin Chang, *Industrial Technology Research Institute*

This paper presents a novel $PM_{2.5}$ detection method. The aerosol sensor, including $PM_{2.5}$ separating, particle charging, ion trap and measurement sections was assembled in a cylinder. When charged particles impact the grounded metal electrode, the electrode will deliver electrical current to the measurement system. The electrical current intensity represents the concentration of particles in the sample. For finding the relationship between the particle mass concentration and the current signal, the correlation between the magnitude of the signal and the particle mass concentration was experimentally investigated where an optical device (DUSTTRAK DRX model 8533, TSI) was employed as a reference of particle mass concentration. The results show that the intensity of the measured current is linearly proportional to the particle mass concentration. The square of correlation coefficient (R^2) is 0.898. The average relative errors of the measured aerosol mass concentration are 10% to 31%.

7LC.13

Challenges in Low-Cost Sensor Calibration: A Case Study on Deployment of Sulfur Dioxide Electrochemical Sensors in an Urban Environment. REBECCA TANZER, Carl Malings, R. Subramanian, Albert Presto, *Carnegie Mellon University*

Low-cost air quality sensors have the potential to greatly increase the spatial resolution of air quality measurements. Low-cost sensors however exhibit cross-sensitivities to gases other than the gas they are built to measure, and sensor response is often dependent on changes in temperature and humidity. In addition, sensor response (e.g., volts/ppb) and the relative importance of cross-sensitivities may change over time. This study examines the precision and bias of low-cost sensors deployed throughout an urban environment over the course of a year, with specific focus on quantifying SO_2 measurement errors near a major point source in a SO_2 non-attainment area.

We deployed Real-time Affordable Multi-Pollutant (RAMP) sensor packages, which use electrochemical sensors for measurement of gaseous pollutants (CO, NO_2, O_3, SO_2). Previous work from this group and others has shown the utility of machine-learning based calibration algorithms to account for electrochemical sensor cross-sensitivities. Some of these algorithms, such as Random Forests, are unable to extrapolate beyond the range of the training dataset, which is particularly challenging for pollutants like SO_2 that often have very low concentrations.

We compare the performance of multiple SO_2 calibration models: (1) laboratory-derived linear regression model and (2) Random Forest model built on co-location of RAMPs with a reference SO_2 monitor at an urban background location; (3) MLR, (4) Random Forest, and (5) Neural Network models built on co-location calibration immediately downwind of a major SO_2 source near Pittsburgh, PA, USA. We held out a portion of the co-location data downwind of the SO_2 source for model testing and validation.

The laboratory regression captures the general trend of SO_2 concentrations for the testing data at the near-source site, but has high error (root mean squared error, RMSE = 14ppb). The random forest models built at the urban background site perform poorly (coefficient of variation of mean absolute error >80%), likely because the training data set that they were built off of did not incorporate SO_2 concentrations >10 ppb. In contrast, all three models built at the high-SO_2 site perform better (mean absolute error, MAE < 4.3ppb) presumably because of a more realistic range of training data.

We tested the spatial transferability of the SO_2 calibrations built at the high SO_2 site by redeploying the RAMPs to new locations. Performance was poorer after redeployment (MAE = 6.7ppb). This appears to be a consequence of the SO_2 calibration models being overfit to the specific SO_2 source near the calibration location, and therefore less generalizable than similar machine learning models for CO and NO_2, which are more variable in time and space. Results for the neural network calibration model generated at the high-SO_2 site demonstrated precision error of 44% and bias error of 38%.

Sensors were deployed and maintained over the course of one year (Spring 2017-Spring 2018). Performance of the electrochemical sensors over the course of the deployment period is to be conducted in order to calculate sensor degradation as a function of time.

7LC.14

Investigating the Performance of a Low-Cost PM Monitor (Dylos) against Dusttrak DRX for Different Indoor and Outdoor PM Sources. MEHDI AMOUEI TORKMAHALLEH, Obaidullah Mohiuddin, Fatemeh Mohammaddezashibi, Madina Obaidullah, Hamed Sharifi, *Chemical and Aerosol Research Team, Nazarbayev University*

Recently, several low-cost, portable optical monitors including Dylos Air Quality Monitor became available in the market and need to be evaluated against the well-reference monitors for public use. United State Environmental Protection Agency (EPA) air sensor workshop recommended several criteria such as linearity of response, the precision of measurements, limit of detection, concentration resolution, response time, interference equivalents, and relative humidity (RH) and temperature influences for the investigation of new air quality sensors. Since the availability of low-cost monitors, researchers have investigated possible correlations with low-cost PM monitors and respective well referenced high-cost monitors. Dylos and Grimm EDM180 showed a medium correlation (R2 = 0.533). Another study was conducted for the correlation of Portable University of Washington Particle (PUWP) monitors with optical and gravimetric PM2.5 reference monitors. The pairwise correlation between them was around (R2- 0.86-0.89). When the test was conducted on eight different sites for measuring PM2.5, the correlation was found to be (R2 = 0.53).

In the present study two instruments were used to examine the air quality. A Dylos DC1700 (a low-cost equipment), was used to measure number concentrations of the particles. Dylos monitors the particle number concentrations in two sizes, larger than 0.5 µm (hereinafter called small size) and larger than 2.5 µm (hereinafter called larger size). The difference between the measurements by Dylos for the two sizes offers the particle number concentration for particle size from 0.5 to 2.5 µm. A DustTrak DRX Model, TSI, USA was employed to measure PM mass concentrations (PM1, PM2.5, PM4, PM10, Total particles). The two monitors were placed near the indoor or outdoor sources with at least one meter away from each other. Dusttrak was zero checked, before starting the experiments. The instruments were operated simultaneously at the same time. Two approaches were employed to compare the Dylos measurements and the Dusttrak data. The difference between Dylos large and small sizes (fine range) was compared with the Dusttrak PM2.5 measurements. Additionally, Dylos large data (coarse range) were compared with the Dusttrak Total PM2.5. Three PM sources including mixed grilling (ground beef meat) and construction particles (Number of measurements=188) generated at faculty residence of Nazarbayev University, outdoor PM (Number of measurements= 9746) in a rural area, Borovoye, Kazakhstan, and smoking particles at Middle East Technical University Northern Cyprus Campus (Number of measurements= 1624) were examined. The operation length were approximately 3hr, 8 days, and 26hr (4 days each 7 hours approximately), respectively. The data for three more sources including beauty shop, construction dust and grilling are being analyzed to be presented during the conference. For Mixed Grilling and Construction source, the correlation coefficient values for fine and coarse fractions were found to be 0.61 and 0.66, respectively, indicating a moderate correlation between Dylos and Dusttrak for this particular source. This moderate correlation could be due to the presence of significant amount of coarse size particles that can be detected by Dylos. A wide range of correlation coefficient values was obtained at four different smoking tests for coarse particles varying from 0.0061 to 0.569. Nevertheless, combining all smoking data, poor correlation values for fine (R2 = 0.17) and coarse (R2 = 0.20) particles were obtained that could be attributed to the presence of PM1 as the dominant size fraction which cannot be completely detected by Dylos. Poor correlation coefficient values were observed for both fine (4Ã—10-5) and coarse (6.1Ã—10-3) particles during the monitoring of outdoor PM in Borovoye, While we are continuing testing different sources until the IAC conference, our conclusion up to this point is that Dylos may show a poor correlation for sources generating particle with major size of PM1. However, it could show an acceptable correlation for sources producing mainly coarse particles.

7LC.15

CFD Analysis of Flow and Particle Behavior in the Performance Evaluation Chamber System for PM Sensor. SUNG-MIN SHIM, Jae-ho Cho, Hyeok Chung, Ki-tai Kang, *Aerosol Research & Technology Plus*

Recently, many studies on the risk of fine dust have been published. Particularly, it has been reported that fine dust particles having a particle diameter of less than 2.5 microns penetrate deeply into the lungs to cause serious respiration and heart-related diseases. As such fine dusts become a common concern worldwide, the World Health Organization, the US EPA, and the European Union are beginning to set up countermeasures. Measurement of fine dust is essential for the fine dust countermeasures. As a method of measuring fine dust, there is a measurement method using a light scattering method and a beta ray absorption method. Therefore, recently, light scattering type fine dust sensor has been actively developed all over the world, and the market related to the fine dust sensor is also growing rapidly. However, the method of evaluating the performance of the fine dust sensor as well as the performance of the fine dust sensor has not yet been clarified yet. Therefore, the fine dust sensor manufacturers evaluate and sell the performance of the fine dust sensor by their own methods. Therefore, a standard performance evaluation system is needed to evaluate the performance of the fine dust sensor in real time under the same test conditions. The fine dust sensor performance evaluation system is divided into a continuous flow type and a batch type according to the test air supply method. The batch type system used in this study has advantages in terms of ensuring uniformity of particle concentration and stabilizing flow since it is not forcibly generated airflow inside the chamber. On the other hand, in the batch system, disturbance of the internal airflow due to the flow generated during sampling of the sensor can affect the spatial uniformity of the particle concentration. Also, measurement device can affect to particle concentration. Therefore, it is necessary to analyze the distribution of the internal airflow and the trend of the particle concentration over time according to the ratio of the internal volume of the chamber and the sampling flow rate of the fine dust sensor. In this study, it is analyzed through computational fluid dynamics. The three - dimensional shape of the chamber and the fine dust sensor was modeled to analyze the flow and particle behavior inside the chamber. In order to simulate the initial flow and particle concentration in the chamber, steady - state analysis was performed under the condition that a constant test flow rate was supplied. The test particles were generated at the test air inlet side in the chamber using the flow analysis results. The particle concentration distribution inside the chamber was predicted. In order to analyze the flow and particle behavior in the chamber by gas sampling of the fine dust sensor, the unsteady flow and particle behavior are analyzed by using the steady state analysis results as initial conditions. The inlet and outlet of the test air in the chamber used the velocity-inlet and pressure outlet conditions, respectively, and the sampling inlet and outlet of the fine dust sensor formed the flow using the fan boundary condition. In order to simulate the decrease of the particle concentration due to the gas sampling of the fine dust sensor, analysis was performed by adding the sink term of the particle to the boundary condition so that the particles in the flow passing through the fan can be removed. The analysis results show that the tendency of airflow in the chamber due to the chamber internal volume and sampling flow rate and the tendency of decreasing the particle concentration by the fine dust sensor.

7LC.16

Toward a More Reliable Optical Smoke Detector: Scattering Matrix Analysis of Fire and Non-fire Aerosol for Classification. QIXING ZHANG, Jia Liu, Jie Luo, Feng Wang, Jinjun Wang, Yongming Zhang, *University of Science and Technology of China*

Point type photoelectric smoke detector, or namely optical smoke detector, is the most common and widely used fire detector in fire protection engineering. This kind of detector senses the light scattered by the smoke entered into the chamber for fire alarm. The optical smoke detector is widely accepted for its features such as low cost, compact, long life, high sensitivity, etc. However, it suffers by the high false alarm rate caused by non-fire aerosols, such as dust, steam (water vapor), cook-generated aerosol, etc. Many efforts have made to develop alternative sensors for building fire alarm, such as temperature sensor, gas sensor, or the combination of these sensors. However, the optical smoke detector still keeps a dominant market share in applications.

Development of a more reliable optical smoke detector is an urgent demand of the fire protection industry. Due to the rigorous requirement of low cost, we constrained the improvement by light scattering characterization for aerosol classification. A better knowledge of the optical properties of the aerosols from fire and nuisances will therefore help to improve the performance of existing detectors, reduce the amount of false alarms, and serve as guideline in the development of the next generation smoke detector. Scattering matrix containing several independent elements, depend on the characteristics of the particles, including size distribution, morphology, and refractive index, has an advantages over non-polarized light scattering for aerosol classification. Here, we present a study of polarized light scattering properties of typical fire and non-fire aerosol through the numerical simulation and experimental measurement of the angular distribution of scattering matrix.

Cement dust and water droplets are selected as typical non-fire aerosols, compared to fresh smoke from several flaming and smoldering test fires. The complete scattering matrix for these aerosols are measured as a function of scattering angle from 5° to 160° at a wavelength of 532 nm by a polarization-modulated scatterometer. Other related characteristics, such as particle size distribution, chemical composition, refractive index and micro morphology are also analyzed. Modelling the scattering matrix of these aerosols considering the detailed morphology are presented and verified by experimental measurement results. Discrimination methods based on the angular distributions of their scattering matrix elements were discussed. The principle guide for detector design by scattering matrix analysis were proposed. A prototype of a smoke detector based on polarized light scattering will also be presented.

7LC.17

The Development of Low-Cost Particle Sensor for Air Quqlity Monitoring. JINHONG AHN, *Innociple Co., Ltd.*

Recently, there has been a widely increasing in the use of low-cost particle sensors for air quality monitor. The most of applications are portable PM monitor and air purifier system. In present, the kind of low-cost PM sensors are IRED type and Laser light scattering type. Several researchers have tested these sensors in the laboratory or ambient environment. In these studies, the sensor generally meets to well at high PM concentrations. But in low PM concentration, these sensors show an underestimated than reference device. In this study, we have developed new low cost PM sensor applied to single particle counting method. Our PM sensor composed of laser diode, focus plano-convex lens, focus mirror and photodiode. This system is similar to general particle counter. So our PM sensor can be measuring particle size and particle counts simultaneously. Thus PM concentrations have made conversion using this information. Our PM sensor can be measure over the 0.5 µm and classify 4 channels. We tested PM sensors against a number of particle mass and number measuring instruments with KCl particles in experimental duct system and ambient aerosols to verify performance. With KCl particles, our sensor meets to very well in the range of 10 to 300 µg/m^3 of PM10 and PM2.5 concentration. The response to KCl particle was also good, with R^2 values in the range of 0.97-0.99.

7LC.18

Using Commercially Available Low-Cost Monitors to Estimate the Hourly Spatial Variability of Particulate Matter Concentrations across a Metropolitan Area. MAURO MASIOL, Stefania Squizzato, David C. Chalupa, Andrea R. Ferro, David Q. Rich, Philip K. Hopke, *University of Rochester Medical Center*

In U.S., the National Ambient Air Quality Standards (NAAQS) set the limit values for six principal "criteria" air pollutants including PM2.5. Data are primarily collected to assess the citywide air pollution concentrations for regulatory purposes. PM2.5 is measured at one or a few urban stations within major cities or in rural locations. This sparse spatial resolution is insufficient to capture the intra-urban spatial variability of air pollution that is driven by the locations and strengths of local sources, the effect of street canyons and complex terrain, and urban heat island effects. Consequently, exposure misclassifications are likely to occur when using these data for epidemiological studies. In addition, NAAQS for PM2.5 requires the attainment of annual or daily limit values. However, recent studies have reported associations between high hourly PM2.5 peaks and mortality/morbidity, particularly cardiovascular events [1]. Consequently, it is important to increase the temporal resolution to capture air pollution peaks responsible of short-term health outcomes.

The accessibility of low-cost sensing for air pollution may be a valuable resource to improve the spatial and temporal resolution of current routine monitoring networks. Low-cost monitors (LCMs) are much less expensive than scientific-grade instruments, physically smaller and lighter (generally portable), collect data with high time resolutions (from few seconds to minutes), require less maintenance, and have low power demands. However, they are not designed to meet rigid performance standards, and they produce data with much less accuracy than scientific-grade instruments. Thus, LCMs require careful calibration and post-processing of data.

Recently, we have used data collected with commercially available LCMs at multiple locations across a metropolitan area of the eastern U.S. (Rochester, NY) during two consecutive winters (2015–2016 and 2016–2017). These monitors (Speck, Airviz Inc., Pittsburgh, PA) were tested under laboratory [2] and field [3] conditions. Data were also used to predict the hourly small-scale variability of PM using sophisticated land-use regression models [4].

The results of a summer/fall sampling campaign (June to October 2017) that essentially completes our dataset to cover all the seasons over three years (2015 to 2017) will be described. Forty-nine LCMs placed in weatherproof cases were deployed outdoors at residential locations in Rochester NY, while another unit was co-located to the NYS DEC air quality monitoring site. Raw data were originally collected at 1 min time resolution. Data were handled to return robust and reliable datasets at 1 h resolution time. Instrumental biases were assessed during 3 days of field co-location with a GRIMM 1.109 aerosol spectrometer pre and post-field deployment. Multiple pairwise analyses were used to investigate the collected data, including coefficient of divergence and signed rank tests of the value distributions.

The data were affected by a large but correctable bias that was caused by the low PM concentrations typically measured in Rochester. However, this main limitation was overcome by a careful instrument calibration and validation of data prior to and after the sampling campaigns to ensure unbiased datasets. Despite the lower accuracy of data, results show that the use of these monitors provides the opportunity for successfully improving the spatial resolution of particulate pollution.

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7LC.19

Measurements of Atmospheric Aerosol Vertical Distribution Using Multi-Rotors Unmanned Aerial Vehicle (UAV) and Portable Aerosol Instruments. ZHIJUN WU, Yishu Zhu, Yong-Hee Park, Kang-Ho An, Min Hu, *Peking University, Beijing, China*

The vertical profile of air pollutants near surface boundary layer is rare but indispensable to bridge the gap between Lidar and satellite measurements and to achieve a more comprehensive understanding of the regional transport of air pollutants. This study investigated the vertical profiles of particle number size distributions, soot concentrations, and trace gases concentrations near surface boundary layer using a multi-rotors unmanned aerial vehicle with a scanning mobility particle sizer and optical particle counter (Developed by Hanyang University, Korea), low-cost sensors (alpha-sense), and MA200 (microAeth). Before conducting the measurements, the influences of rotating multi-rotors on the aerosol sampling were tested using flow visualization technique (tuft test). With increasing length of the vertical aerosol inlet, the turbulence caused by rotating multi-rotors became to be weak. The optimized length of the sampling inlet was fixed to be 1.5 meter. The field measurements were carried out in a rural site, located between Beijing and Tianjin cities. The vertical profiles of particle number size distribution, soot particle mass concentration, and meteorological parameters were measured. The preliminary results showed that new particle formation took place a higher latitude associating with an increased ozone concentration. The detail data analysis will be given in the presentation.

7LC.20

A Guideline for the Application of the Shinyei PPD24NS Low-Cost Dust Sensor for Air Quality Monitoring. Michael Canu, BORIS GALVIS, Ricardo Morales Betancourt, Omar Ramirez, Malika Madelin, *Universidad De La Salle, Colombia*

There is increasing demand for low-cost dust sensors for air quality monitoring applications. The Shinyei PPD24NS is one to the most used devices but there is few work that establishes its performance conditions and characteristics. Consequently, its use has produced mixed results in terms of accuracy, precision and repeatability especially when they are employed while in motion. Our work aims at filling this gap by providing insight on the sensor operation, its limitations, the influence of air flow and noise sources. This work presents a guideline on supply voltage filtering, assembly and data treatment, aimed to improve the sensors' shortcomings for future applications.

7LC.21

Continuous Field Calibration of Low-Cost PM2.5 Sensor Networks. Kyle Alberti, GEOFF HENSHAW, Georgia Miskell, Hamesh Patel, Jonathan Taylor, David Williams, *Aeroqual Ltd*

The availability of low-cost PM2.5 sensors has enabled large numbers of such devices to be deployed in a variety of ad-hoc networks which have the potential to provide new insights into the distribution of this pollutant at community and street level. However new methods to calibrate and validate such data are needed that are commensurate with the low-cost nature of such networks.

We report on the field application of a simple, continuous calibration technique to a hierarchical PM2.5 network located in California featuring a small number of PM2.5 regulatory instruments (“proxies”) and a much larger number of low-cost devices. The technique calculates slope and offset for the low-cost devices from the mean and variance of the time-averaged distribution proxy data over a similar time interval.

We explore the effect of different types of proxies on the calibration accuracy and the benefits and limitations of the approach.

7LC.22

Application of Low-Cost Sensors for the Monitoring of Air Quality by Bicycle. ERICK KILL, Paulo Saldiva, Luiz Pereira, *University of São Paulo*

Air pollution is a serious public health problem around the world. Studies that investigate the relationship between air pollution and human health are fundamental to management that aims to promote urban development and quality of life. Air quality monitoring systems are an early premise for such studies, especially so that it focuses on spatial assessment.

In this sense, low-cost sensors expand new possibilities for monitoring air quality. The protocols and monitoring sensors are extremely new, justifying the need for research to integrate technologies and improve environmental information systems. An important point for improving air quality monitoring is the sharing of environmental data from different sources (public and private companies), a real-time system in order to take advantage of data from different sensor networks.

Currently, monitoring by networks of fixed stations are managed by official entities related to the environment. This monitoring has high reliability in data generation and is capable of accurately measuring a wide range of air pollutants using traditional instruments. However, the disadvantages of such measurement systems are their large dimensions, high cost and complex maintenance.

There are some basic limitations to the approaches used to control and publish air quality data: the spatial resolution of pollution sampling is low, making it necessary to use mathematical models to estimate concentrations of pollutants in unmonitored areas of metropolitan regions ; Current observations of concentrations do not reflect actual exposures experienced by humans due to the spatial heterogeneity of pollutant concentrations and the mobility patterns of individuals.

Trying to contribute to minimize this identified gap, the objective of this present project is the implementation of low cost networks for air quality monitoring, using Internet Protocols of Things (IoT) protocols, models for evaluation and calibration of these equipments. of personal and local evaluation, selected as an object of agreement, based on the analysis data of the air quality network of the Environmental Company of the State of São Paulo (CETESB), remote sensing data, analytical tests (trace gases), resulting in an air quality network model.

The research method adopted will be the use of statistical models and data collection in the field (remote sensing and micro controlled equipment on board). As some of the expected results of the work are: results with local and spatial variability of air quality (real time), precision adjustments against currently adopted models, development of WebGIS portal (room of situation) and availability of results in application platform mobile (app).

7LC.24

Fine-scale Spatio-temporal Variation in Particulate Matter in a Small Wood-burning Town Revealed by a Network of Continuous Low-cost Sensors. Ian Longley, Gustavo Olivares, Sam Edwards, GUY COULSON, *National Inst of Water and Atmospheric Research, New Zealand*

Following a co-location study, 15 monitoring nodes, based on the Plantower 3003 dust sensor, were deployed across a small New Zealand town for a minimum of 19 days in winter 2016. Rangiora has previously been identified as a town where wintertime concentrations of particulate matter breech the National Environmental Standard of 50g m-3 over 24 hours, and emissions are dominated by wood combustion for home heating. The location of the town on a coastal plain in the lee of a mountain range leads to complex air flows especially at dusk when nocturnal boundary layers form and emissions peak.

The sensors were initially co-located with a TEOM-FDMS operated by the regulatory authority. PM2.5 concentrations were then measured every minute at the 15 locations distributed across the town (area approx. 17 km2, pop. 17,000) for 19 days (and at some of the sites for longer). This was supported by the deployment of three temporary automatic weather stations on the periphery of the town. A further co-location study was conducted at the end of the campaign.

All 15 sensors reported valid data throughout the campaign. The co-location study revealed high correlation between the Plantower sensors and the TEOM-FDMS with very stable performance. No interferences were detected (e.g. related to air temperature or humidity). The sensitivity of each individual sensor varied but was sufficiently stable to be adjusted for with a simple linear function.

On average the data revealed a large degree of spatial variation in concentrations across the town. The spatial variation was not consistent over time but highly complex. A tendency for concentrations to peak earlier in the east and later in the west was observable and broadly consistent with shifts in wind direction. Inspection of the time series indicated that some sites were subject to temporary elevations in concentrations (anomalies with respect to typical or larger-scale patterns) that imply localised near-source and plume-strike impacts.

7LC.25

Theoretical Analysis of a High-Pass Electrical Mobility Filter. NIC SURAWSKI, Spyros Bezantakos, Konstantinos Barmpounis, Andreas Schmidt-Ott, George Biskos, *University of Technology Sydney*

A recent focus in aerosol research has been the development of lightweight, low cost and portable devices for sensing airborne particulate matter. Advances in the field (e.g. Bezantakos et al. (2015) and Surawski et al. (2017)) have shown that it is possible to size-segregate nanoparticles (< 50 nm in diameter) by designing a precipitator (also referred to as a High-Pass Electrical Mobility Filter; HP-EMF) constructed from electrostatic dissipative materials. Whilst effective size segregation has been demonstrated with this technique, theoretical analysis is required to ensure that the mechanism of sensing rests on firm grounds.

In this study, we mirror the approach used by Knutson and Whitby (1975) in their analysis of the differential mobility analyser, Stolzenburg (1988) in his analysis of the tandem mobility differential analyser and Biskos et al. (2005) in their analysis of the differential mobility spectrometer to derive the transfer function for the HP-EMF. Given its cylindrical geometry, and well-defined electric field, analytic solutions to the non-diffusing and diffusing transfer functions can be obtained. A key feature of our analysis is that diffusion does not degrade the performance of the HP-EMF unlike other instruments such as the differential mobility analyser. This result is achieved since with a reduction in size (or increase in electrical mobility) the reduced residence time in the HP-EMF compensates for the increase in a particle's diffusivity. As such, our theoretical analysis suggests that the HP-EMF has certain design advantages compared to other aerosol sizing devices.

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7LC.27

The Performance Evaluation System of Low-Cost Air Quality Sensors in Taiwan. Yen-Ting Li, CHIA-WEI CHANG, Yi-Cyun Yang, Jiunn-Haur Shaw, Yeuh-Bin Wang, *Industrial Technology Research Institute*

With the tremendous advantage and wide application of low-cost $PM_{2.5}$ sensors in the Internet of Things (IoT) network, many citizens in Taiwan had installed personal $PM_{2.5}$ sensors and shared their monitoring data to the public. However, the data quality of commercially available low-cost sensors is varied, and the misuse of data might arise unnecessary worries. To systematically evaluate the performance of low-cost $PM_{2.5}$ sensors, Taiwan EPA (Environmental Protection Administration) works with ITRI (Industrial Technology Research Institute) on the building of the corresponding evaluation platform. The platform includes two testing environments, one under the real outdoor environment (field test), and the other under the well-controlled environment (lab test). Data from $PM_{2.5}$ sensors are compared with USEPA FEM (Federal Equivalent Method) instruments installed in the platform, and parameters including intra-model variability, data recovery, accuracy（bias error）, and linear correlation coefficient (R^2) of $PM_{2.5}$ sensors could be investigated by the field test station. Additional parameters such as precision, interferents, detection limit, and drift could be investigated by the lab test station. The lab test station also covers the evaluation of sensors performances under extreme environments (temperature, humidity, $PM_{2.5}$ concentration). We state in detail in this report the hardware design and testing protocol of the platform, and testing results of some $PM_{2.5}$ sensors. We anticipate this platform could help the control of data quality of $PM_{2.5}$ sensors and thus improve the air quality monitoring in Taiwan.

7MG.1

Study of the PM2.5 Growth Processes in Two Key Regions of China. Jinjin Sun, Mingjie Liang, JIANLIN HU, Qi Ying, Hongliang Zhang, *Nanjing University of Information Science & Technology*

Regional atmospheric environment pollution problems have become increasingly prominent in China in recent years, due to large amount of air pollutant emissions with the rapid economic development, the rapid growth of energy consumption and intensified urbanization. Specifically, the regions of Beijing-Tianjin-Hebei (BTH) and the Yangtze River Delta (YRD) are among the most economically developed and populated areas in China but also these regions are suffering extremely heavy air pollution. Fine particulate matter (PM2.5) is a major environmental problem in these two regions and greatly affects public health. A few case studies observed that PM2.5 could grow quickly in the two regions. The factors and processes that affect the growth processes still remain unclear.

In this study, we analyze the dynamic accumulation of PM2.5 using hourly concentration in the two regions. We focus on the PM2.5 growth processes from 35 to 150 µg/m3. We analyze all the growth processes in four years of 2013-2016 in 19 cities in the BTH and 21 cities in the YRD region. PM2.5 rising rates (PMRR) and dynamic growth duration (T) are calculated to illustrate the characteristics of the growth processes.

The results show that Beijing and Nanjing had 148 and 75 PM2.5 growth processes, respectively, during 2013-2016. The 4-year average PMRR in Beijing and Nanjing, is 5.28 µg/(m3.h), and 3.75 µg/(m3.h), respectively. Clear difference is observed between cities in BTH and YRD. Further analysis of the growth rates, associated meteorological conditions, chemical components of PM2.5 will be performed to investigate the controlling factors for different growth processes in different cities and regions.

7MG.2

Mercury Stable Isotope Compositions of PM2.5 in Chinese Cities. HONGMEI XU, Ruoyu Sun, Junji Cao, *Xi'an Jiaotong University*

Atmospheric pollution by fine particulates and mercury (Hg) in emerging economies is a serious environmental concern. Here, we present Hg concentrations and isotope compositions during one month (January 2014) of 24-hour integrated fine particulate matter ($PM_{2.5}$) samples from four large Chinese cities (Beijing, Changchun, Chengdu and Hong Kong) to identify Hg sources and transformation processes. Mean concentrations of $PM_{2.5}$ (171±62 μg m^{-3}) and $PM_{2.5}$-bound Hg (1.3±1.1 ng m^{-3}) in Chengdu were the highest. Overall, $PM_{2.5}$ samples were characterized by moderately negative δ^{202}Hg (-1.08±0.64‰, 1σ, n=64), slightly negative Δ^{199}Hg (-0.13±0.28‰, 1σ, n=64) and insignificant Δ^{200}Hg (0.03±0.05‰, 1σ, n=64). On average, δ^{202}Hg of $PM_{2.5}$ was the highest in Chengdu (-0.74±0.67‰, 1σ, n=29), followed by Beijing (-1.11±0.26‰, 1σ, n=17) and Changchun (-1.60±0.45‰, 1σ, n=18). $PM_{2.5}$ from Beijing showed the most negative Δ^{199}Hg (-0.31±0.40‰, 1σ, n=17) that was significantly lower than Changchun (-0.12±0.21‰, 1σ, n=18) and Chengdu (-0.02±0.15‰, 1σ, n=29). Coal combustion and cement production were identified to be the dominant sources of $PM_{2.5}$-bound Hg in these cities, with additional Hg sources from non-ferrous metal smelting in Chengdu. Besides, Hg emissions from biomass burning were evident during short periods. The negative Δ^{199}Hg and near-unity slope of Δ^{199}Hg vs. Δ^{201}Hg in $PM_{2.5}$ from different cities indicate that the $PM_{2.5}$-bound Hg was extensively photo-reduced in the local atmosphere following emission from sources.

7MG.3

Size-segregated Chemical Components of Aerosol Particles in Hefei, China. ANNA LI, *Laboratory of Atmospheric Physico-Chemistry, Anhui Institute*

To investigate the characteristics of aerosols in typical pollution episodes, water-soluble inorganic ions,including anions (NO_3^-,SO_4^{2-},F^-,Cl^-) and cations (NH_4^+,Na^+,Ca^{2+},Mg^{2+},K^+) in 8 size-segregated particle fractions, are collected by an Anderson sampler from Dec.2016 to Jan.2017 in Hefei. The results of chemical composition analysis showed that secondary water soluble ions NO_3^-,SO_4^{2-},NH_4^+ (SWSI) composed more than half the total ions, and are mainly found in fine particles (aerodynamic diameters less than 2.1 mm), while Ca^{2+} and Mg^{2+} contributed to a large fraction of the total water-soluble ions in coarse particles (aerodynamic diameters greater than 2.1 mm and less than 9.0 mm). The SWSI showed a bimodal size distribution with the peak mass concentration of particles shifted from 0.43–0.65 µm on clear days to 0.65–1.1 µm on lightly polluted days and to 1.1–2.1 µm on heavily polluted days. NH_4^+ played an important role in the size distributions and the formations of NO_3^-,SO_4^{2-}. Heterogeneous reaction is the main formation mechanism of NO_3^- and SO_4^{2-}, which tended to be enriched in the coarse mode of aerosol. In this study the average NO_3^-/ SO_4^{2-} mass ratios decreased from clear (3.7 and 3.8, respectively) to LP (3 and 3.6, respectively) and to HP (2.6 and 2.9, respectively) days for both fine and coarse particles. The mass ratio suggesting that Local sources played a more important role in the formation of particles .Meteorological conditions contributed to influence the secondary formation and regulate the size distributions of SWSI. Short-distance transport, low wind speed and high RH were highly responsible for the formation of the pollution event.

7MG.4

Primary Sources and Secondary Formation of Organic Aerosols in Diadema, São Paulo, Brazil. DJACINTO MONTEIRO DOS SANTOS, Luciana Rizzo, Patrick Schlag, Samara Carbone, Paulo Artaxo, *University of São Paulo*

The Diadema city is one of the 39 municipalities within São Paulo Metropolitan Area (SPMA), very impacted by industrial and vehicular emissions, but also near to preserved Atlantic forest areas. This combination of different anthropogenic and biogenic sources results in complex physicochemical processes that culminate in the formation of secondary aerosols and ozone. An aerosol and trace gas monitoring station was operated at Federal University of São Paulo Campus, in Diadema, from 15 November 2016 to 15 March 2017, spring to summer in south hemisphere. Aerosol chemical composition was analyzed using an Aerodyne ACSM instrument. Measurements of aerosol properties like size distribution, number concentration, scattering and absorption coefficients, and gas phase (NO2, SO2 and O3) concentrations were taken. During campaign, the average concentration of PM_1 was 10.1 (7.2) $\mu g\ m^{-3}$. On average, the chemical composition of submicron aerosol is dominated by organics (55%), followed by equivalent black carbon (eBC), sulfate, nitrate and ammonium, with 15%, 15%, 8% and 6%, respectively. Average NO_2 and SO_2 concentrations were 13 ppb and 0.6 ppb, respectively, while ozone peaks 33 ppb at the middle of the day. Using Positive Matrix Factorization (PMF), the organic component was divided into different factors, identified as oxygenated organic aerosol (OOA), biomass burning organic aerosol (BBOA) and two components of hydrogenated-like organic aerosol (HOA). The OOA factor, dominated by m/z 44, was described as aged particles associated with secondary organic aerosols (SOA). The respective mass spectrum shows a good correlation with typical low volatile OOA mass spectrum. Moreover, time series of OOA factor correlates with time series of secondary species (SO_4, O_3 and NO_3) and its average diurnal profile presents maximum concentration during afternoon, which evidences the role of photochemical activity in the formation of SOA in Diadema. The two HOA factors showed similar mass spectrum characterized by a hydrocarbon-like structure typically associated to vehicle exhaust emissions. The time series of these factors has high correlation with primary vehicular emission tracers and its diurnal profile presents peak concentrations during the local morning rush hour. The average contributions of OOA, HOA (sum of two HOA factors) and BBOA factors to total OA mass concentration were 44%, 41% and 15%, respectively.

7MG.5

Contributions of the N2O5 Heterogeneous Hydrolysis Reaction to the Nitrate Formation in the North China Plain (NCP) During Wintertime: A Case Study. LANG LIU, Guohui Li, *Institute of Earth Environment, Chinese Academy of Sciences*

Although stringent emission mitigation strategies have been implemented in China since 2013 to improve the air quality, heavy haze with high levels of fine particulate matters (PM2.5) still frequently engulfs the North China Plain (NCP), China. Observations show that the nitrate aerosol has played an increasingly important role in the heave haze formation, constituting a major component of PM2.5. The N2O5 heterogeneous hydrolysis reaction is the most important pathway of the nitrate formation during nighttime or even dominates the nitrate formation during heavy haze episodes with weak sunlight and high humidity. The reaction is dependent on temperature, relative humidity, and aerosol constituents, including sulfate and organic matters. In the present study, the WRF-CHEM model is applied to quantify the contribution of the N2O5 heterogeneous hydrolysis reaction to the nitrate formation and investigate the effect of organic coating on the hydrolysis reaction during persistent haze pollution episodes from 10 to 27 February 2014 in NCP. The WRF-CHEM model generally performs well in simulating the temporal variations and spatial distributions of air pollutants concentrations against observations at ambient monitoring sites in NCP. The simulated diurnal variations of inorganic aerosol species are also well consistent with the measurements in Beijing. Simulations show that on average during the episodes, the nitrate aerosol contributes around 25% of PM2.5 mass concentrations in NCP. The N2O5 heterogeneous hydrolysis reaction accounts for about 34% of nitrate concentrations, playing an important role in the nitrate formation and contributing appreciably to PM2.5 mass concentrations. The organic coating effect on the N2O5 hydrolysis reaction considerably suppresses the nitrate formation, reducing the nitrate concentration by more than 10% during heavy haze days and also improving the nitrate simulation against the measurement. Our results highlight the importance of the nitrate aerosol to the heavy haze formation in NCP and the N2O5 heterogeneous hydrolysis reaction to the nitrate formation. Further studies need also to been conducted to evaluate the organic coating effect on the nitrate formation.

7MG.6

Lahore Smog – Componential Analysis, Causes and Effects. ZULFIQAR ALI, Irfan Zainab, Zona Zaidi, Komel Ahmad, Syed Turab Raza, Saira Khan, Rida Ahmad, Khadija Aziz, Mubashir Ahmad, Sidra Safdar, Zaheer Ahmad Nasir, Ian Colbeck, Nimra Afzal, *University of the Punjab, Lahore, 54590, Pakistan*

South and East Asia is the region where 99 percent human reside in areas with poor air quality where $PM_{2.5}$ levels greatly exceed the WHO limits of 25 µg/m³. With the annual average $PM_{2.5}$ levels of 101 µg/m³, Pakistan is enlisted as one of the worst countries in terms of air pollution with an annual mortality rate of more than 22,600 deaths per year in 2005, of which more than 800 were children under five years of age. Ambient levels of particulate matter have been reported by many researchers to be manifolds higher than the WHO recommended limits and there has been very little if any work done on improving the air quality of urban areas.

The last two years forecast of Lahore has been hazy with dense fog and smoky at start of November each year. At first the smog was considered a normal though unexpected event but by the second year, there were increasing complaints of burning in the eyes and breathing difficulties.

The smog persisted and the visibility was reduced to almost zero. People were warned to stay indoors and to limit any outdoor activities if any. They were advised to wear masks when outdoors and to keep washing their eyes with water from time to time so as to minimize the risk of exposure to the deadly haze surrounding the city.

The data for current smog episodes was collected from real time continuous ambient air monitors DRX (8533TSI), Aeroqual (500) with sensors Sulfur dioxide, Nitrogen dioxide; Ozone, and Carbon Dioxide along with metrological parameters like humidity, wind speed and temperature by Kestral (4000) Weather Station. A volumetric sampler with 40 liter per minute was used to assess further chemical and biological analysis.

November 2016 was characterized with high level of critical pollutants, which in general, were attributed to geographical location of the Lahore city in high crop burning area, high vehicular and population density. The smoggy condition was prevailed for about 14 days (October to November 2016), and 15 days in 2017 with onset a week earlier. In 2016 the situation persisted for almost two weeks and reported cases for Acute Respiratory Illness increased by 19 percent and 67 percent in 2017 for same period. Due to breathing difficulties and lung damage increased hospital admissions were evident for the reason that of smog episodes after harsh exposure. These complications may lead to premature deaths as its proved in studies that thousands of deaths in Europe, Asia and the United states have been linked to effects of smog.

Upon monitoring the air of the city, it was found to be laden with extremely high levels of VOCs, and particulate matter with some concentration of NO_x while ozone and SO_x were negligible. Lead was also found to be in alarming concentrations. The major sources attributed to the buildup of these pollutants included the increase in motor vehicles and industrial units in and around the city while burning of agricultural crop residue in India at a massive level was also highlighted by NASA to be the main culprit. Combined with high atmospheric pressure, increased humidity and thus low wind speed the pollutants were unable to disperse thereby affecting the health of the residents. This smog episode can be considered a warning bell for the government agencies and the public since these incidents may recur if the sources are not reduced and strong initiatives for clean air are not taken on time.

7MG.7

Characteristics of Atmospheric Ammonia and Its Relationship with Vehicle Emissions in Shanghai. Ruyu Wang, XINGNAN YE, *Fudan University*

Atmospheric ammonia can not only neutralize sulfate and nitrate to form secondary inorganic aerosols but also favor aqueous oxidation of SO_2 and NO_x, which plays an important role in haze formation in East China. In this study, long-term measurements of NH3 concentrations were implemented at urban, suburban, and tunnel sites in Shanghai, the largest city in East China. The average monthly ammonia concentrations at the urban site varied from 3.7 ppb to 14.5 ppb and exhibited the highest levels in summer and lowest levels in winter, indicating that the biological emissions and agriculture in the surrounding areas are important contributors. The suburban NH_3 levels were significantly higher in autumn compared to those at the urban site, indicating the important contribution of agricultural activities. Regardless of the season, the concentrations of NH_3 at the tunnel site remained almost constant. On average, the tunnel NH_3 level was three times higher than that of the nearby urban site, indicating strong vehicle NH_3 emissions in the tunnel. The tunnel NH_3 levels on weekdays were comparable to those on weekends, a result that was in agreement with the daily average traffic volume. It was estimated that the vehicle emissions contributed 12.6-24.6% of the atmospheric NH_3 in the urban area of the city and 3.8-7.5% of the total for the whole city. Our results suggest that regulation and control of NH_3 emissions from traffic should be considered in order to mitigate severe haze pollution during wintertime in the megacities of China.

7MG.8

Secondary Organic Aerosol Production over Seoul, South Korea, during KORUS-AQ. BENJAMIN A. NAULT, Pedro Campuzano-Jost, Douglas Day, Jason Schroder, Bruce Anderson, Andreas Beyersdorf, Donald Blake, William Brune, John Crounse, Ronald Cohen, Joost de Gouw, Jack Dibb, Josh DiGangi, Glenn Diskin, Alan Fried, Greg Huey, Christoph Knote, Kara D. Lamb, Taehyoung Lee, Sally Pusede, Joshua P. Schwarz, Paul Wennberg, Armin Wisthaler, Jose-Luis Jimenez, et al., *University of Colorado-Boulder*

Secondary organic aerosol (SOA) is rapidly produced over and downwind of urban areas, causing important effects on health, visibility, and climate. At this time, only a few megacities have been well characterized for urban SOA production. In this study, we utilize observations from the NASA DC-8 over Seoul, South Korea, during the NASA/NIER 2016 KORean United States-Air Quality (KORUS-AQ) study to quantitatively investigate the relative importance of transported OA (and SOA precursors) to Seoul versus the influence of local emissions of SOA precursors.

From the airborne observations, we find that SOA production (normalized to excess CO) over Seoul is higher than that observed over other urban areas around the world, including even locations in China. However, when SOA production is normalized to excess CO2, the SOA production across urban areas shows more similarity, due to China having higher CO emissions relative to SOA precursor than other areas. Results from an Oxidation Flow Reactor (OFR), that was flown on the NASA DC-8, shows that the absolute potential SOA over Seoul is a factor of 3 higher than over the West Sea, indicating local emissions are dominating the SOA production over this urban region, similar to results for more isolated urban regions like Los Angeles and Mexico City. Also, we find that the potential SOA produced in the OFR during morning overpasses of the city are similar to the observed ambient SOA produced later in the day, indicative of photochemistry dominating the SOA production over this urban region. Furthermore, correlations of SOA with short-lived products (formaldehyde and peroxy acyl nitrate, which have lifetimes of less than 4 hours in this region) from oxidation of hydrocarbons, along with correlation of SOA with ozone, indicate that the SOA is being locally produced from photochemistry of local hydrocarbon emissions. We corroborate this finding through calculations of potential SOA productions from observations, finding that short-lived hydrocarbons (OH chemical lifetimes of less than 1 day) dominate (~90%) the SOA production budget. Finally, local dominance of SOA precursors is further supported with source analysis results from WRF-Chem / FLEXPART, using NO_2 as a surrogate for short-lived hydrocarbons (given their similar lifetimes). This study highlights the role of local hydrocarbon emissions with rapid photochemistry dominating the SOA production budget in the Seoul urban region.

7MG.9

Influence of Diwali Fireworks on Air Quality and Aerosol Optical Properties over a Mega City Delhi. SATEESH M., Vijay Kumar Soni, Raju P.V.S., *India Meteorological Department*

Ten days intensive observational studies of aerosols properties and air quality have been carried out at mega city Delhi, the national capital of India. During the Diwali festival fire crackers are burnt extensively in Northern part of India. The Skyradiometer data from Skynet-India along with ambient air pollution data were analyzed for the period November 09-18, 2012. Aerosol radiative forcing and heating rate was calculated using SBDART model.

Aerosol Optical Depth (AOD) value increased to as high as 2.55 and 0.45 for the wavelengths 340 and 1020 nm respectively. Single Scattering Albedo (SSA) increased to 0.996 at 500 nm and 0.863 at 1020 nm on the Diwali. Asymmetry Parameter (ASY) increased to a maximum of 0.79 for the shorter wavelength at 340 nm and 0.6 is reported at the higher wavelength 1020 nm. The real part of the Refractive index was observed to be 1.625 at 1020 nm and 1.4467 at 340 nm. The imaginary part of the refractive index decreased to -0.01766 at 1020 nm and -0.00031 at 340 nm. It has a good correlation of 90% with observed AOD and MODIS data, standard deviation of 0.31 and a RMSE of 0.17 for the Diwali period. Heating rate of 1.8 oC.day^{-1} in the 1km layer, 0.4oC.day^{-1} in the 10 km layer was observed. There is a 28W.m^{-2} radiative forcing trapped within the atmosphere for the first day of the diwali and a 30W.m^{-2} is trapped on the second day of the Diwali. And it is increased to 34 W.m^{-2} for the next three days (SBDART-Model). The concentration of PM10 and PM2.5 was reported as maximum of 2641 µg.m^{-3} and 1876 µg.m^{-3} respectively on the Diwali day. Concentration of SO2 varied between 13 to 88 µg.m^{-3} during the Diwali period. A highest of 109 ppb surface ozone is reported in the night time 23:00 IST, where the NOX is 63.7 ppb and NO2 is 23.2 ppb.

7MG.10

Characteristics and Formation Mechanism of Nitrate during Haze Events in Beijing. QINGCHENG XU, Shuxiao Wang, Yang Hua, Jiming Hao, *Tsinghua University*

Water-soluble inorganic ions (WSI) is major components of PM2.5 in Beijing in recent years. Since year 2015, sulfate concentrations in PM2.5 has gradually decreased owing to the effective control of coal combustion. However, the contribution of nitrate to PM2.5 displayed a significant increase during haze events in Beijing. In this study, a highly time-resolved online analyzer (Monitoring for AeRosols and Gases, MARGA) was employed to measure the WSI in PM2.5 in Beijing from 5 February to 15 November, 2017. Three typical haze events during this period were selected and investigated. During our campaign, the mass ratio of nitrate to sulfate changed from 2.4 to 2.67 when the air pollution aggravated from slightly polluted (150>AQI>100,115>PM2.5>75) to moderately polluted (AQI>150, PM2.5>115). This study used mass concentration of nitrate/sulfate to CO(gas) to exclude the effects of planetary boundary layer in four selected haze event. The results show that time-series of PM2.5 is significantly correlated with nitrate (with a correlation coefficient of 0.53), while it is not correlated with sulfate. During heavy pollution episodes in winter, nitrate concentrations increased from 7.5 µg/m3 to 45.6µg/m3, while sulfate increased from 4.2µg/m3 to 20.1µg/m3, indicating that nitrate is a more important driver for the growth of PM2.5. Nitrate also dominates the increase of WSI in the pollution episodes in autumn, with a concentration of 52.5µg/m3, and contributes up to 67% of WSI. The average ratio of NH4+ to SO42- was 1.62 in autumn, much higher than that in summer (0.86). One of the reason is that the emission control of coal combustion in Beijing and surrounding areas results in an NH3-rich and SO2-lean atmosphere, which promoted the formation of ammonium nitrate. Even in summer, when the meteorological conditions are much more suitable for the photochemical reaction of ammonium sulfate than ammonium nitrate, there are still significant amount of ammonium nitrate formation in the night with variations in temperature and relative humidity. This study indicates that nitrate is becoming the most important component of WSI in PM2.5 and is driving the rapid growth of PM2.5 concentrations during heavy pollution episodes. Therefore, more efforts shall be made to reduce the nitrogen oxide and ammonia emissions in North China.

7MG.11

Effects of Aqueous-phase and Photochemical Chemistry on Winter Haze Formation and Evolution in Beijing, China.

TAO MA, Fengkui Duan, Hiroshi Furutani, Michisato Toyoda, Takashi Kimoto, Lidan Zhu, Yongliang Ma, Kebin He,
Tsinghua University

In recent years, severe hazes with high $PM_{2.5}$ concentrations have been serious problems in China due to the rapid economic growth and urbanization. To better understand the severe winter hazes in Beijing, a suite of strengthened observations was conducted in Tsinghua University from December 21, 2015 to January 8, 2016 with hourly-based continuous gas and particle measurements including a single particle mass spectrometer (ATOFMS). Four continuous severe haze episodes were observed and $PM_{2.5}$ concentration varied from 2.7 $\mu g\ m^{-3}$ to 506.3 $\mu g\ m^{-3}$ during the campaign. We classified air quality into three types: clean ($PM_{2.5} \leq 75\ \mu g\ m^{-3}$), dry-haze ($PM_{2.5} > 75\ \mu g\ m^{-3}$ and $RH < 80\%$) and wet-haze ($PM_{2.5} > 75\ \mu g\ m^{-3}$ and $RH \geq 80\%$). Based on ART-2a method, we classified all single particles into 7 groups: OC-day, OC-night, K-rich, Na-rich, K/Na-rich, K/Na-CN and Metal-rich. During clean and dry-haze periods, organic compounds were dominant, while SNA (sulfate, nitrate and ammonium) increased quickly to be major components during wet-haze periods. The oxidation ratio of sulfur and nitrogen increased with RH, indicating the importance of aqueous reaction on secondary inorganics formation during severe hazes. OC/EC showed bimodal diurnal variation, consistent with OC-day and OC-night particle types. The phenomenon indicated the effect of photochemical and aqueous chemistry on secondary organic aerosol formation in daytime and nighttime, respectively. Meteorological conditions also have a strong impact on haze formation. High $PM_{2.5}$ concentrations usually appeared under the condition of low wind speed and high humidity, which were in favor of the pollutants accumulation and secondary transformation.

7MG.12

Determination of the Emission Sources of Particulate Matter in Queretaro (Mexico). SARA ERIKA OLIVARES, Dara Salcedo, Harry Alvarez-Ospina, Carina Aguillon-Vazques, *National University of Mexico*

Queretaro is located in the center of Mexico, 270 km north of the City of Mexico Metropolitan Area and is one of the cities with highest economic development in recent years, coupled with rapid population growth (30% in the last 15 years) and an expansion of industrial areas within and near the city. As a result, there has been an increase in the amount of pollutants emitted into the atmosphere, including particulate matter (PM). Given that PM is one of the pollutants with greatest impact on human health, it is important to identify its sources in order to implement regulations to control its ambient concentration.

PM_{10} and $PM_{2.5}$ were collected at three sites in Queretaro during 2014 and 2017. The concentration of trace elements in the samples was determined using Inductively Coupled Plasma Mass Spectrometry (ICP-MS). The results were analyzed using the EPA´s Positive Matriz Factorization (PMF) model in order to identify the main PM sources in the city of Queretaro.

Preliminary results show that PM_{10} has a cortical origin, while the $PM_{2.5}$ is mainly of anthropic origin, as expected. A more detailed analysis will be presented showing the characteristics, relative contributions, and time series of the source identified. Comparison of the data at different periods and sites will be used to describe the temporal and spatial variability of the PM and trace elements concentrations.

7MG.13

First Measurements from Smear Beijing Station: New Particle Formation in Urban Beijing and Source Apportionment of Atmospheric Pollutants. CHAO YAN, Juha Kangasluoma, Federico Bianchi, Tommy Chan, Biwu Chu, Lubna Dada, Kaspar Rudolf Dällenbach, Yueyun Fu, Xucheng He, Liine Heikkinen, Heikki Junninen, Yiliang Liu, Yiqun Lu, Qingxin Ma, Pekka Rantala, Yonghong Wang, Gan Yang, Rujin Yin, Ying Zhou, Joni Kujansuu, Tuukka Petäjä, Yongchun Liu, Lin Wang, Jingkun Jiang, Markku Kulmala, *University of Helsinki/BUCT*

New particle formation (NPF) contributes a significant fraction to the total atmospheric particle load and affects the air quality. NPF proceeds via gas-to-particle conversion, which is governed by the availability of precursor vapors and existing particle surface area that the vapors can condense onto. In an urban environment, they are strongly affected by the local sources and micrometeorology. To obtain a comprehensive view on the processes governing air quality and NPF, long-term continuous measurements are needed. Continuous measurements allow monitoring of response of the atmosphere to the various forcers, which the short-term campaign-type measurements cannot observe.

Because of recent rapid urbanization of the developing countries such as China and India, severe air quality problems and haze episodes have taken place in large cities, such as Beijing and Delhi. The exact mechanisms responsible for the worst haze episodes still remain unclear, but they are linked to at least increased emissions from the industry, traffic and heating. To monitor the air quality in urban Beijing area, a new SMEAR Beijing station has been established close to the western third ring road at the Beijing University of Chemical Technology.

The current measurement capabilities of the station include inorganic trace gases, NO3 radicals, nitrous acid (HONO), volatile organic compounds, low-volatility vapors (H2SO4 and highly oxygenated organic compounds), particle and ion size distributions, particle chemical composition and meteorological parameters. The measurement has been started since Jan.12 2018, and will be continued throughout the year. We will present our results with two main focuses: First, the driving mechanism of NPF in Beijing, especially those cases during highly polluted conditions; Second, comprehensive analysis of source apportionment on VOC emissions, oxidation pathways, and aerosol chemical characteristics.

7MG.15

Black Carbon Source Apportionment In Delhi during Winter. UMESH C. DUMKA, Suresh Tiwari, D.G. Kaskaoutis, S.D. Attri, Vijay Kumar Soni, P.D. Safai, Narendra Singh, N. Mihalopoulos, *ARIES Nainital*

Urban areas in the developing countries are major sources of carbonaceous aerosols, especially for black carbon (BC) that constitutes the most efficient absorbing aerosol, pointing out the need for detailed assessment of the levels and source apportionment close to the source. In the current work, we present a multi-instrument research campaign which was performed in Delhi, India during December 2015 – February 2016 aiming at exploring the pollution levels and the BC source apportionment due to fossil-fuel (BC_{ff}) and wood burning (BC_{wb}) using the "Aethalometer model" approach. The database consists of continuous measurements of BC mass concentrations, scattering, absorption, and extinction aerosol coefficients, along with the intensive aerosol properties like single scattering albedo (SSA), extinction and absorption Ångström exponents (SAE and AAE, respectively), air pollutants (CO, NO_x, O_3) and meteorological observations.

The results show very high pollution (PM_{10}, $PM_{2.5}$, CO, NO_x, and O_3) levels, while the daily-mean BC mass concentration ranging from 3.2 μg m^{-3} to 59.9 μg m^{-3}. The very weak winds along with the shallow boundary layer favor the accumulation of the pollutants near the ground resulting in high BC mass concentrations. The daily-averaged Absorption Ångström Exponent (AAE), the BC_{ff}/BC and BC_{ff}/BC_{wb} ratios varied between 1.1 – 1.5, 0.5 – 0.9, and 1.1 – 9.9, respectively due to changes in the BC emission rates, variations in the relative emissions from fossil-fuel and wood-burning sources and the mixing processes in the atmosphere. The mean BC_{wb} contribution to total BC mass was estimated at 28% at 880 nm, while at 370 nm, the BC_{wb} accounts for the 44% of the BC emissions, highlighting an important biomass-burning component within the urban environment. The BC_{ff} and BC_{wb} components also exhibit remarkable diurnal patterns with maximum concentrations in the morning and evening/night hours and lower around noon primarily driven by the boundary-layer dynamics. The BC_{ff}/BC fraction maximizes during the late night-to-morning hours, while the BCwb exhibits higher contribution in the evening hours, pointing out increased emissions from wood and waste-material burning for heating purposes.

7MG.16

Chemical Properties of PM 2.5 and Their Potential Source in Urban Background of Delhi, India. MANOJ KUMAR, Fasiur Rahman, Divesh Bhatia, Gazala Habib, *IIT Delhi*

A rapid economic growth and high energy demand in developing countries such as India have resulted in the massive discharge of atmospheric particulate matter (PM). PM concentration in Delhi and other metro cities is often found to exceed the Indian National Ambient Air Quality Standards (NAAQS) and recent studies have identified PM as one of the key public health risks, particularly in urban regions such as Delhi. In the past three years, the PM concentration in Delhi significantly exceeded the permissible limits during the autumn season (October and November) when smog-like conditions prevail. This has been qualitatively attributed to the burning of biomass/crop residuals in areas adjoining Delhi. However, very few quantitative studies have focused on the chemical composition of PM2.5 to obtain the source of PM. The present study focuses on PM2.5 measurement and its chemical characterization as carbonaceous aerosol [Elemental carbon (EC) and Organic Carbon (OC)], trace elements during summer and autumn season in Delhi and its relation with the regional meteorology. PM2.5 samples were collected on Teflon and Quartz filters using a dual stage multi-stream sampler equipped with a cyclone separator (URG Corporation, USA) and two filter holders operated at 10 LPM using critical orifices. The samples were collected from June 2017 to November 2017. The mass collected on backup quartz filters was used for the artifact correction. During the study period, the 24-hour mean concentration of PM2.5 was observed as 71.9 ± 4.2 (n=29) and 179.1 ± 10.8 (n=22) μg m^{-3} for summer and autumn season, respectively, i.e., the PM2.5 concentration in the autumn season was twice that of the summer season. Interestingly, it was found that the PM2.5 concentration during the episodic smog was ~10 times higher than the NAAQS standards, and also eight times higher compared to the non-episodic days. Further, the chemical composition of trace element and OC/EC will be analyzed by Energy Dispersive X-ray Fluorescence (ED-XRF) and Thermal Optical Transmittance (TOT) analyzer. A source apportionment study of PM2.5 using the Positive Matrix Factorization (PMF) model also will be conducted and discussed.

7MG.17

Implementation Effect and Countermeasures of the "Air Pollution Prevention and Control Action Plan". WENKANG GAO, Guiqian Tang, Mengtian Cheng, Dongsheng Ji, Zirui Liu, Tao Song, Liang Li, Junke Zhang, Yuesi Wang, *Inst. of Atmospheric Physics, Chinese Academy of Sciences*

The National Council promulgated the "Air Pollution Prevention and Control Action Plan" ("action plan") in 12 September, 2013. To study the different regionals air pollution control effects in China after the "action plan", $PM_{2.5}$ concentration was analyzed in 36 monitoring sites of the Campaign on atmospheric Aerosol Research network of China (CARE-China) between 2013 and 2016. To research the reason of change of $PM_{2.5}$ concentration in different regions in China, the concentrations of SO_2 and NO_2 in 74 cities were analyzed, which was released by the China Ministry of Environmental Protection. The results show that the PM2.5 concentration was reduced by 9-35 µg/m^3 in different regions in China. SO_2 and NO_2, the main precursors of particulate matters, decreased 37.1% and 6.3% in the ground level, respectively. However, the NO_2 column density was decrease ~20% significantly, indicating the strong emission reduction of elevated point sources. The observations in Beijing showed that the concentrations of PM_1 and $PM_{2.5}$ were decreased by 5.7 and 0.2 µg/m^3, respectively. However, the concentration of $PM_{1-2.5}$ increased 27.9% and NH_4^+ was the main contributor with 16.2% increasing in $PM_{1-2.5}$. During implementation of SO_2 and NO_x emission reduction measures, the issue of fossil fuel combustion NH_3 leak should be paid attention. Meanwhile, it should still be strengthened that the control of vehicle emissions on the ground.

7MG.18

Individual Exposure of PM2.5 and Health Risk Assessment of Heavy Metals in Nanchong Traffic Police. GUO JIALING, Li Youping, *China West Normal University, Nanchong, Sichuan*

In order to explore the situation of $PM_{2.5}$ accepted by traffic police in Nanchong and the potential risk of heavy metal elements in PM2.5 by breathing into human body. On July 12,2013~July 21,we carried out on-site online monitoring of individual exposure of traffic police in Nanchong, and we also collected $PM_{2.5}$ samples from air by using filter membrane. Then, we analyzed the composition of heavy metals in $PM_{2.5}$ which had been collected . Finally, we made the health risk assessment according to the analytic result. The result showed that the average individual exposure concentration of $PM_{2.5}$ accepted by traffic police in Nanchong during the monitoring period was 74.8μg/m^3 which was slightly lower than the national secondary standard daily average concentration of 75μg/m^3. The correlation analysis showed that the wind speed had a negative correlation with the exposure concentration of PM2.5 ,as well as, the correlation of temperature, relative humidity and other meteorological parameters to the exposure concentration of PM2.5 was poor. The order of the concentrations of heavy metals in PM2.5 in Nanchong city was: Fe> Zn> Mn> Pb> Sb> Ni> Cu > Cr> Co> V. The study found that Mn had a serious non carcinogenic risk to traffic police in Nanchong which with a non-carcinogenic risk index of 2.48. While the Cr had a high risk of carcinogenesis in Nanchong and should pay attention to it.

7MG.20

Aerosol Sources and Processes in Winter in Beijing: Insights from Aerosol Mass Spectrometry. YELE SUN, Zifa Wang, Pingqing Fu, Qingqing Wang, Wei Du, Weiqi Xu, Jian Zhao, Wei Zhou, *Institute of Atmospheric Physics, CAS*

Winter has the worst air pollution in a year in the megacity of Beijing, yet our knowledge on the sources, formation mechanisms and evolution of aerosol particles is far from complete. Here we present the results from several winter campaigns that were conducted in urban Beijing from 2011 using an Aerosol Chemical Speciation Monitor and a High Resolution Aerosol Mass Spectrometer. The sources of organic aerosol (OA) have been fully characterized using positive matrix factorization and multilinear engine. The composition and variations of primary OA (POA), e.g., from coal combustion, cooking, and biomass burning emissions, and different types of secondary OA (SOA), and their roles in severe haze pollution are elucidated. Further, the effects of photochemical and aqueous-phase processing on SOA composition, oxidation states, and evolution processes are characterized. In addition, real-time aerosol particle composition measurements were also conducted at two different heights on a meteorological tower by using two aerosol mass spectrometers. The vertical differences in aerosol composition and sources, and its interactions with boundary layer dynamics will be presented.

7MG.21

Evaluating Effects of Stubble Burning in Punjab and Haryana on the Air Quality of Delhi and National Capital Region.

RAKESH KUMAR, Sanjeev Goyal, Gulia Sunil, Hemant Bherwani, *NEERI*

Deteriorating urban air quality in Delhi and National Capital region (NCR) is one of the prime topics of discussion. There are many distinctive features of Delhi which impact air pollution like uncontrolled sources of pollution in its surrounding perimeter (where city regulations do not apply, and where they apply, are not followed stringently), a number of unregulated and unaccounted sources within the city, unfavourable geographic location and regional meteorology, with windy and dusty conditions during summer and foggy weather with limited ventilation and mixing during winter. At the onset of winter, during the Months of October-November every year, a thick blanket of smoke and fog covers the northern states including Delhi. Hazy weather is witnessed during these winter months which may have been caused by pollution emissions during Diwali celebrations period and smoke generated from burning of agriculture stubble during a few overlapping or subsequent weeks. However, there has been no conclusive study available that adequately determines the dynamics and movement of the pollutants that come towards Delhi due to burning of stubble (paddy crop) residue in states like Punjab and Haryana.

Agricultural stubble burning emits significant quantity of air pollutants like NOx, SO_2, CO, NH_3 and particulate matter. The current study is trying to evaluate the contribution of pollution from the stubble burning in the states of Haryana and Punjab in the air quality of Delhi and NCR. Ambient air quality monitoring with respect to major air pollutants, viz. PM_{10}, $PM_{2.5}$, SO_2 and NO2 is carried out during the stubble burning period in Punjab and Haryana States. Chemical profiling is also done under the studyA total of seven sites were selected for ambient air quality monitoring, two in Punjab: Patiala and Sangrur; two in Haryana State: Karnal and Rohtak; and three in Delhi: Pitampura, Sarojini Nagar and Nariana. Twelve hours sampling is done, twice a day, from 8am to 8pm and 8pm to 8 am.

Episodic days are also monitored during these two months. High pollution loading was observed during the month of November. It is also observed that, in general, the monitored sites breach the National Ambient Air Quality Standards (NAAQS), set at 100 $\mu g/m^3$ and 60 $\mu g/m_3$ for PM_{10} and $PM_{2.5}$ respectively, even during the normal days and are much higher during the episodic days. During the analysis, it was also observed that local sources around monitoring station influences the air quality significantly. The meteorological parameters are monitored in Ludhiana (Punjab), Rohtak (Haryana) and Nariana (Delhi). Winds are mostly observed in calm condition during the study period. This may be indicating towards a very low possibility of movement of long transport of pollution and more contribution of local sources in pollution level. The current study comprising of weather monitoring, ambient air quality monitoring, chemical characterisation and source profiling, reveals interesting facts about the correlation between Delhi's pollution level and stubble burning in the states of Haryana and Punjab and the same is discussed in the detailed paper.

7MG.22

Characteristics of Submicron Aerosols in Summer of Beijing: Particle Size, Density, Hygroscopicity, and Mixing State.

SONG GUO, Min Hu, Dongjie Shang, Zhuofei Du, Jing Zheng, Renyi Zhang, *Peking University*

To characterize the air pollution of North China Plain of China, CAREBEIJING-2013 field campaign (Campaigns of Air quality REsearch in BEIJING and surrounding region) was conducted in summer of 2013. Submicron aerosols were measured at an urban site PKU (Peking University, 39°59’21”N, 116°18’25” E) from July 28th to September 31st 2013. A suite of integrated instruments was used to measure the size distribution, effective density and hygroscopicity of ambient particles. The chemical composition of submicron particles were measured by using an Aerodyne High-Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS) . The average $PM_{2.5}$ concentration was 73.0±70.7 μg m^{-3} during the measurement. The particulate pollution showed distinct 4-7 days cycles controlled by the meteorological conditions. Each cycle started with low $PM_{2.5}$ mass concentrations (<20 μg m^{-3}), since the air mass was from relatively clean mountainous area. The particle number concentrations were high, but and the sizes were small (<30 nm) at this stage, which can be explained by the new particle formation. In the succeeding days, both the particle mass and size continuously increased. The $PM_{2.5}$ concentration increased rapidly by >60 μg day^{-1}, and the particle mean diameter grew to >100 nm. It is interesting to note that the mean diameters showed similar trend to PM2.5 mass concentrations, indicating the particle pollution attributed to the growth of the newly formed small particles. During the measurement, the average particle densities are between 1.3-1.5 g cm^{-3}, indicating organics and sulfate were dominant in the particles. The densities of smaller particles, i.e. 46 nm, 81nm, showed single peak at 1.3-1.5 g cm^{-3}, indicating the particles are internal mixed sulfate and organics. While the 150nm and 240 nm particle densities exhibited bimodal distribution with an additional small peak at ~1.1 g cm^{-3}, which is considered as external mixed organic particles or aged soot particles. The particle hygroscopic growth factor for all the measured sizes at RH of 90% showed bimodal distribution, attributing to external mixed organics (or aged soot) and internal mixed organics and sulfate. Both the density and HGF were higher than Tijuana, but similar to Houston. PMF (Positive Matrix Factorization) model was deployed to quantify the contributions of different mixing state particles. Internal mixed organics and sulfate were dominant in the ambient particles in Beijing.

7MG.24

The Influence of Gaseous Pollutants and Particulate Matter Concentration on New Particle Formation in Beijing.

RUJING YIN, Yiqun Lu, Chao Yan, Juha Kangasluoma, Tommy Chan, Biwu Chu, Chenjuan Deng, Yueyun Fu, Xucheng He, Yiliang Liu, Xiaohui Qiao, Pekka Rantala, Yonghong Wang, Mo Xue, Gan Yang, Ying Zhou, Joni Kujansuu, Tuukka Petäjä, Yongchun Liu, Lin Wang, Jingkun Jiang, Markku Kulmala, *Tsinghua University*

In the past decades, high concentrations of particulate matter and gaseous pollutants were observed in China, especially in the most populated and industrialized regions. To improve the air quality, the government has upgraded or closed a number of unqualified enterprises and replaced coal with electricity and natural gas for residential heating in Jing-Jin-Ji region, which led to significant reductions in coal-burning-related pollutants, such as sulfur dioxide (SO2) and PM2.5.

Such changes may have profound influences on the concentration of gas-phase sulfuric acid (H2SO4). On the one hand, the source of H2SO4 was affected from two counteracting aspects: the decreased SO2 but enhanced photochemistry due to less light extinction in the clean boundary layer. On the other hand, the sink of SO2, commonly known as condensation sink (CS), also dropped significantly. The changes in H2SO4 could in turn affect new particle formation (NPF) in the atmosphere, which potentially contributes a large fraction of the number concentration of atmospheric aerosol particles. Simultaneously, the declined CS should also play an important role in regulating the occurrence of NPF.

To understand the non-linear effect of pollution reduction on the formation of H2SO4 and newly-formed particles, we conducted a field campaign at the Beijing University of Chemical Technology located in downtown Beijing. The measurement started on Jan.12, 2018. We deployed a NO3--based CI-API-TOF to measure sulfuric acid and some highly oxygenated organic molecules (HOMs) and electrical mobility spectrometers to characterize particles size distribution down to ~ 1 nm. We will present the measurement details and illustrate the effects of pollution reduction on the concentration of H2SO4 and the NPF by comparing to the data collected in 2016 and 2008 when Beijing hosted the Summer Olympic games.

7MG.25

Gaseous Nitrated Phenols as a Potential Source of OH Radicals in Beijing. XI CHENG, Qi Chen, Ying Liu, Tong Zhu, *Peking University*

Nitrated phenols (NPs) are a family of aromatic compounds having both nitro and hydroxyl groups connecting to a benzene ring. These species are important because of their phytotoxicity in agriculture and forestry and their contribution to atmospheric oxidative capacity. Gaseous NPs in the atmosphere had been mainly measured by using off-line methods. In this study, we deployed a chemical ionization time-of-flight mass spectrometer equipped with reagent nitrate ion source in Beijing during 2016 to 2017. The accuracy of mass calibration was within 10 ppm for the measurement periods, and NP species were unambiguously identified in the mass spectra. The concentrations of NPs were calibrated by using standard permeation tubes. Sampling wall losses were also determined. High concentrations of gaseous NPs were observed in Beijing (sometimes hundreds of pptv in total), which came from both primary emissions and secondary production. Nighttime enhancements of the NP concentrations often occurred. Moreover, the occurrence of haze in Beijing correlates well with the strong enhancements of dinitrophenol concentrations. During the haze events, the dinitrophenol concentrations alone may go above 150 pptv, possibly explained by aqueous phase reactions. The results suggest that the photolysis of gaseous NPs can be an important source to form atmospheric oxidant in the heavily-polluted urban environment.

7MG.26

Sources and Transformations to Atmospheric Aerosols in Winter: A Carbon and Nitrogen Isotopic Study in Beijing.

QIAN YU, Mo Xue, Di Wu, Lei Duan, Jingkun Jiang, Shuxiao Wang, *Tsinghua University*

Stable carbon and nitrogen isotopic compositions can provide complementary information about sources and transformations of atmospheric aerosol and have long been conducted in several sites in developed countries. However, little is known in China and no extensive studies have been focused on stable carbon and nitrogen simultaneously. Here, we report ^{13}C and ^{15}N natural abundance (δ^{13}C, δ^{15}N) for $PM_{1.0}$ and $PM_{2.5}$ collected in Beijing during November to December 2017, together with nitrate (NO_3^-), ammonium (NH_4^+), and organic matter contents from two online aerosol chemical composition monitors using liquid chromatography and mass spectrometry, respectively. The objective was to test whether δ^{13}C and δ^{15}N can be used to reveal sources and transformations of atmospheric aerosol. We found that δ^{13}C in $PM_{2.5}$ and $PM_{1.0}$ ranged from -26.9‰ to -22.9‰ (ave. 24.5 ± 0.7‰) and -28.3‰ to -25.7‰ (ave. 27.4 ± 0.9 ‰), respectively. It indicates that coal combustion and vehicle emission (or second formation) contribute significantly to organic composition of $PM_{2.5}$ and $PM_{1.0}$ in Beijing. δ^{15}N of $PM_{2.5}$ had a wide range (1.64‰ -15.2‰, ave. 10.2 ± 3.1‰) and had distinct values during the clean day (1.64‰ -7.54‰) and polluted period (10.2‰-15.2‰). δ^{15}N were not significantly related to aerosol mass concentrations or the NO_3^- and NH_4^+ contents, but showed positively correlation with the ratio of NO_3^--N/(NO_3^--N+NH_4^+-N). It suggests that primary emission from coal combustion contributes to atmospheric aerosol in the clean day, but second formation from photochemical processing of NO_x was the major source during the polluted period. This study, explicitly recognizing the different sources and transformations of atmospheric aerosol in different size range and during different episodes, established stable isotope method for regional source apportionment of ambient particulate matter.

7MS.1

Production of Homogeneous Particles by Controlled Neutralization of Electrosprays. Antonio Carrasco-Munoz, Elena Barbero-Colmenar, Eszter Bodnar, Jordi Grifoll, JOAN ROSELL-LLOMPART, *Universitat Rovira i Virgili*

Electro-hydrodynamic atomization (EHDA) of liquids, or electrospray, is a promising way of generating uniformly sized micro- and nano-drops, as building blocks for the production of nanoparticles and nanostructured coatings. In this technique, a liquid meniscus is electrified to form a microscopic jet that spontaneously breaks up regularly, resulting in uniformly sized drops. However, EHDA has not yet been implemented industrially much, due to the lack of robust atomization methods that can mass-produce uniform droplets. One of the challenges is to overcome the high electrical charge carried by the droplets, which leads to several issues. Specifically, as solvent evaporates from droplets containing a non-volatile solute, the charge concentrates till a limit (Rayleigh limit) is reached, at which they explode, distorting the shape of the resulting particles and the size distribution uniformity.

To overcome this drawback, we have explored experimentally and numerically the implementation of controlled sources of ions of opposite polarity to the electrospray droplets in order to neutralize them. The simulation includes a 3D Lagrangian model for droplet motion, a droplet-ion neutralization kinetics according classical electrostatic charging theories, and a gas velocity field obtained with COMSOL 5.2. Additional features are the coalescence of droplets with low electrical charge of the same or opposite sign, and droplet evaporation.

When ions are injected from the counter electrode zone under the influence of a gas velocity field, controlled neutralization of the droplets can be achieved and thus Coulomb explosions can be avoided. The forces that drive the droplets progressively change from electrical to gas drag as the droplets progress from the needle to the counter electrode. Experimentally, we find that the aerosol extraction efficiency is dramatically improved when ions are injected into the electrospray.

7MS.2

Ultrafast Conversion of Ag Nanoagglomerates into Ag2S Nanodots via Photoionization of Ag in Thiol Droplets. Bijay Kumar Poudel, Kyung-Oh Doh, JEONG HOON BYEON, *Yeungnam University*

Photoinduced ultrafast assembly of Ag_2S nanodots with surface thiolates was achieved in a single–pass gas stream configuration. Ag nanoagglomerates were converted into aligned Ag_2S nanodots without hydrothermal reaction, separation, or purification procedures. The proposed route to fabricate hybrid nanodroplets containing Ag nanoagglomerates and 1–hexanethiol resulted in electrostatic interactions between Ag surfaces and thiol groups to assemble Ag_2S nanodots. Photoirradiation (185–nm wavelength UV) onto the nanodroplets induced electron detachments from Ag via photons (photon energy: 6.2 eV) reaching the Ag (work function: 4.5 eV) surfaces. The positively charged Ag surfaces interacted with the negatively charged surrounding thiol groups, resulting in the formation of Ag_2S nanodots. Continuous photoirradiation for 6.4 s resulted in complete phase transfer; thus, inducing isolation of the nanodots (i.e., resulting in an aligned structure of the nanodots without random aggregation) by conjugated surface thiolates. The nanodots were stably dispersible for near–infrared–radiation–induced fluorescence bioimaging without significant cytotoxic effects; furthermore, merging the nanodots with TiO_2 nanoparticles significantly enhanced photocurrent generation under simulated solar irradiation. The photoinduced ultrafast assembly demonstrates a new feasible safe–by–design platform to continuously manufacture photoresponsive nanodots without optimization concerning chemically efficient and environmentally benign concepts.

7MS.3

Fabrication of Graphene Encapsulated Silicon Composites from Graphene Oxides and Waste Silicon Sludge for Lithium Ion Batteries. HEE DONG JANG, Sun Kyung Kim, Hankwon Chang, *Korea Institute of Geoscience & Mineral Resources*

Over 40% of high-purity silicon (Si) ingot is consumed as sludge waste consisting of Si, silicon carbide (SiC) particles and metal impurities during Si wafer slicing in semiconductor fabrication. Recovery of Si from the waste Si sludge has been a great concern because Si particles are promising high-capacity anode materials for Li ion batteries (LIBs).

In this study, we report a novel aerosol process that not only extracts Si particles but also generates Si-graphene (GR) composites from the colloidal mixture of waste Si sludge and graphene oxide (GO) at the same time by ultrasonic atomization-assisted spray pyrolysis. The effects of the operating temperature, concentration of Si sludge powder and GO in the colloidal mixture on the particle properties were investigated. The morphology of the as-formed Si-GR composites looked like a crumpled paper ball and the average size of the composites varied from 0.6 to 0.8 µm with variation of the process variables. The Si-GR composites exhibited very high performance as Li ion battery anodes in terms of capacity, cycling stability, and Coulombic efficiency.

7MS.4

Aerosol Chemical Vapor Deposition of Nanostructured Thin Films for Lithium-Ion Battery Negative Electrodes.

CLAYTON KACICA, Louis Wang, Tandeep Chadha, Pratim Biswas, *Washington University in St Louis*

Electrochemical energy storage has become increasingly important in recent years due to increasing numbers of electric vehicles in use and the expanded deployment of intermittent renewable energy. Improvements in current battery technologies, such as increased longevity and higher energy density, are necessary for these new applications. Lithium-ion batteries (LIBs) are the most promising candidate for use in these applications due to their many advantageous properties.

Current research is focusing on the development of new electrode materials and electrode morphologies. Metal oxides, such as tin dioxide (SnO_2), have been the focus of much work for utilization as negative electrodes due to their high theoretical capacities. However, these materials undergo a large volume expansion when charged that can lead to rapid capacity fade or battery failure. Using nanostructured morphologies, such as nanospheres, nanotubes, and nanorods, has been shown to significantly reduce the instability of these electrode materials. Using aerosol techniques, we can synthesize nanostructured metal oxide materials in a way that is both scalable and economically feasible.

One such technique is aerosol chemical vapor deposition (ACVD), in which a vapor phase organometallic precursor is fed into a reactor where it undergoes thermal degradation to for metal oxide monomers. Nucleation and condensational growth of particles occur before the particle deposit onto a heated substrate and sinter into films of various morphologies. Using various system parameters, the characteristic times for the processes occurring in the reactor can be controlled and used to determine the final morphology of the deposited material. Because ACVD can be used to deposit directly onto a current collector, the post-processing steps usually required for electrode fabrication are eliminated.

In this work, highly oriented columnar nanostructured SnO_2 electrodes were fabricated using ACVD and utilized as high-capacity negative electrodes in LIBs. The nanostructured electrodes exhibited an initial specific discharge capacity of 1433 mAh g^{-1} and after 100 galvanostatic charge-discharge cycles at a charge rate of 1 C retained a specific discharge capacity of 445 mAh g^{-1}. However, when increasing the charge rate to 2 C significantly more capacity fade is observed resulting in specific discharge capacity of 251 mAh g^{-1} after 100 cycles. In order to enhance the capacity retention of the electrodes, a thin layer of TiO_2 was applied to prevent irreversible parasitic reactions from occurring. The TiO_2 coated SnO_2 electrodes exhibited a specific capacity of 497 mAh g^{-1} after 100 charge-discharge cycles at a rate of 2 C, with coulombic efficiencies over 99% after the first cycle. Diffusion studies were conducted to ensure that the TiO_2 coating was not impeding the movement of Li^+ ions. The study showed that the diffusion coefficient of Li^+ was not impeded for coatings of TiO_2 that was less than 26 nm.

7MS.5

Stability and Control of the Electrospray Cone-Jet Mode. Gabriel Garcia-Soriano, Santiago Martin, Jose L Castillo, PEDRO L GARCIA-YBARRA, *Universidad Nacional de Educacion a Distancia - UNED*

Electrospraying is a valuable technique to prepare nanostructured layers by aerosolization and deposition of nanoparticles on a collector. This method has been used for the formation of catalytic coatings with a very large active surface to be used as PEM fuel cell electrodes. The sprayed liquids are inks prepared by stirring solutions of catalytic nanoparticles in alcohols that are impelled to the electrospray nozzle by a syringe pump at a constant flow rate. To get a high degree of homogeneity in the coating, the spraying is done in the cone-jet mode which guaranties the emission of a continuous jet of monodisperse droplets that, after the alcohol evaporation stage, leads finally to an aerosol of solid charged nanoparticles driven by the electric field towards the collector. The bottle neck of the method is the small yield of the electrospray, which compel to work with the maximum allowed flow rate to minimize the deposition time. However, large values of the flow rate render unstable the cone-jet mode when the voltage difference between the nozzle and the collector surpass the borders of the “stability island”. This region has a wedge shape that shrinks for large flow rates where the cone-jet mode is easily destabilized leading to either a multijet mode or an oscillating mode.

A control system has been developed to retain the electrospray in the cone-jet mode. The system is based on a continuous measurement of the current at the nozzle due to the emission of charged droplets. The determination of the cone-jet stability borders is cumbersome due to the hysteresis displayed by the electrospray in the transition between this mode to and from the other working regimes. The boundaries of the stability island of an ethanol electrospray have been characterized and the emitted current measured in the different regimes with high temporal resolution. The current shows abrupt jumps when the electrospray mode changes. This characterization has been used to set up a proportional-integral-derivative PID control system to maintain the electrospray in the cone-jet mode for long periods of operation.

7MS.6

Novel Aerosol Method for the Fabrication of Si-MWCNT-C Composite Spheres as Anode Materials for Lithium Ion Battery. HANKWON CHANG, Chan Mi Kim, Sun Kyung Kim, Dae Sup Kil, Hee Dong Jang, *Korea Institute of Geoscience and Mineral Resources*

Silicon has attracted extensive attention due to its high theoretical capacity, low discharge potential and non-toxicity as anode materials for lithium ion batteries (LIBs). Here, we suggest a novel aerosol method for the fabrication of Si-MWCNT-C composite spheres as a high-efficient anode material for lithium ion batteries. Si particles were interlinked by MWCNT within droplets sprayed from aqueous glucose solution with Si and MWCNT particles via spray drying method, and then the Si-MWCNT-glucose particles were carbonized at a muffle furnace. The spherical Si-MWCNT-C composites was successfully obtained. The particle size ranged from 2.1 to 3.3 µm in a geometric mean diameter with respect to the concentrations of Si and MWCNT in the precursor. The electrochemical performance was conducted with the Si-MWCNT-C composites as an anode for LIBs. The Si-MWCNT-C composites exhibited very high performance in terms of capacity and cycling stability. After 100 cycles, the capacity of Si-MWCNT-C with 0.4 wt% of MWCNT was maintained to 1042 mAh/g.

7MS.7

Copper Nanoparticle-based Films Fabricated by Spark Discharge Deposition for Surface-Enhanced Raman Spectroscopy. MOHAMED ABD EL-AAL, Takafumi Seto, Yoshio Otani, *Kanazawa University*

Copper nanoparticles were fabricated and deposited on glass substrate by spark discharge of copper rod under atmospheric pressure. The average diameter of the as-prepared Cu primary particles was measured by the TEM to be 3.7 ± 1.2 nm. Thermal annealing of the film induced the growth of the Cu grains from 27 nm at room temperature to 54 nm at 200oC. A water solution of dye molecule (crystal violet) with concentration of 10-6 to 10-8 M was dropped on the prepared Cu substrate. Raman signals from dye molecule were detected and their intensities changed according to spark time, annealing temperature and dye concentration. Significant increase in the Raman scattering signal of dye molecule was observed in the film fabricated at 30 min deposition time with post-annealing temperature of 200°C for 1h. This substrate provides a maximum SERS intensity with a detection limit of 10-8 M, which in the single molecule level with an enhancement factor of 3.9×103. The relationship between the SERS performance of the substrates and their surface morphologies was investigated by the SEM and EDX.

Keywords: Cu nanoparticles; Spark discharge; SERS; Crystal violet.

7MS.8

Using Aerosol-based Analytical Methods for the Synthesis of Functional Nanomaterial Colloids. DE-HAO TSAI, *National Tsing Hua University*

We present a systematic study on the developments of aerosol-based analytical methods for the synthesis of functional nanomaterial colloids. Electrospray-differential mobility analysis is employed to study dis-assembly/de-aggregation of metal organic framework, quantification of nanosheet graphene oxide colloids, protein-silver nanoparticle interactions, ligand–nanoparticle interactions for silica, ceria, and titania nanopowders, and orthogonal analysis of functional gold nanoparticles for biomedical applications. Physical size and colloidal stability of nanomaterials are tunable by the adjustment of environmental conditions. Complementary physical, microscopic and spectroscopic characterization methods are incorporated to the study, allowing for a concept of applications of nanomaterial colloids involving the control of particle size and homogeneity and further proving the capability of in-situ semi-quantitative analysis in a variety of aqueous formulations.

7MS.9

Size-Controlled Synthesis of Pd Doped TiO2 Catalyst in a Flame Aerosol Reactor (FLAR) for Oxygen Removal from Carbon Dioxide Enriched Combustion Exhaust Gases. SUNGYOON JUNG, Pratim Biswas, *Washington University in St Louis*

To mitigate the level of CO_2 emitted from the coal-fired combustion systems, an oxy-coal combustion system has been developed as a promising technique to effectively capture CO_2 in power plants. The captured CO_2 can be either sequestered [1] or reused for enhanced oil recovery (EOR) [2] or converted to value added products [3]. Although a highly concentrated CO_2 stream was achieved in the combustion exhaust gas (~63%), it cannot be directly applied for EOR or sequestration because of a residual concentration of oxygen (O_2) (~3%), which is greater than the requirement for EOR (<100ppmv) [4], and the strict requirement to prevent corrosion in the transportation pipeline (10 ppmv) [5]. To overcome this shortcoming, catalytic O_2 removal system with hydrocarbons has been recently proposed. In this study, we developed a one-step synthesis method of Pd doped TiO_2 catalysts for an efficient O_2 removal by catalytic methane (CH_4) oxidation reaction. To achieve this, we first synthesized Pd doped TiO_2 catalysts with different Pd loading (1.3, 5.5, and 11.7%) in using flame aerosol reactor (FLAR). Flame synthesis has been extensively used as a gas phase technique that can produce homogeneous nanoparticles and can be scaled up for high throughput production. Second, we developed a differential fixed-bed reactor to test the O_2 removal performance of the catalysts. The activity of synthesized catalysts was tested at temperatures ranging between 25 and 500 °C and under atmosphere pressure. When near stoichiometric condition ($O_2/CH_4=2$) was applied for the catalytic activity tests, enhanced conversion of O_2 (~40%) was obtained at 400 °C with Pd (1.5%) doped TiO_2 catalyst compared to that (~22%) with only TiO_2 catalyst. In addition, O_2 conversion increases with increasing Pd doping. The enhanced catalytic activity of Pd-doped TiO_2 catalysts for O_2 removal was supported by the structural properties of catalysts which are increasing rutile phase confirmed by X-ray diffraction and well-dispersed Pd clusters on TiO_2 nanoparticles (~12 nm) revealed by transmission electron microscopy and energy-dispersive X-ray spectroscopy. This study highlights a new insight into an effective O_2 removal by using flame-synthesized Pd-doped TiO_2 catalysts to decrease the O_2 concentration in flue gas emitted from oxy-coal combustion system.

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7MS.10

Investigation of the Role of Charging on the Particle Growth during Combustion in Spray Flame Aerosol Reactor.

SUKRANT DHAWAN, Girish Sharma, Pratim Biswas, *Washington University in St Louis*

The precise control of particle formation and growth in combustion processes is important for a wide range of applications and their environmental implications. In combustion systems, such as a flame aerosol reactor, a large number of ionized species are produced because of chemical and thermal ionization mechanisms (1) with concentrations as high as 10^{10} #/cm^3. These highly concentrated ions collide with particles and the particles collide with each other and coagulate to form larger particles. These ion-particle interactions can significantly impact the particle formation and growth processes that eventually affect the properties of the synthesized particles. Therefore, it is crucial to study the impact of charging to better understand the particle evolution and growth in the combustion systems, and for precise control of the properties of flame synthesized particles.

In this study, the aim is to investigate the role of charging on the particle growth. To achieve this, TiO_2 nanoparticles were synthesized in the spray flame aerosol reactor using TTIP as precursor and the in-situ charge distribution characteristics of the synthesized particles were investigated using a tandem differential mobility analyzer coupled with a condensation particle counter. These measurements were conducted at different heights above the burner to obtain the particle size and charge distribution a function of their residence time. The experimental measurements were then coupled with the theoretical aerosol dynamic equation to predict particle growth dynamics. In the model, both ion–particle interactions (Fuchs' charging theory) and particle–particle interactions were taken into account to simulate simultaneous charging, and coagulation of particles (2). The effect of charge on particle growth was examined at different flame condition and precursor concentrations.

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7MS.11

Aerosol-assisted Synthesis of a Columnar TiO2 Electron Transport Layer for Application in Photovoltaics. ROBIN WHEELUS, Shalinee Kavadiya, Pratim Biswas, *Washington University in St. Louis*

With the threat of worsening global climate change and the increase in world-wide energy demand, the need for cheap renewable energy is higher now than ever. Perovskites, since their introduction into this application in 2009, have grown in power conversion efficiency from less than 4% to more than 22% in recent years. As researchers work to counteract perovskite's natural tendency to break down from exposure to air and water, it is important to continue to investigate new possible methods for improving the cell's efficiency. This research aims to enhance cell efficiency by improving the electron transport layer (ETL) of the cell. 1-Dimensional structures have been shown in the past to have superior electron transporting properties because of their minimization of randomness of the electron's path and straight 1-dimensional transport from perovskite absorber layer to the charge collector electrode. These structures have been created from a wide variety of methods in many shapes and sizes. Our approach is to use an aerosol technique known as Aerosol Chemical Vapor Deposition (ACVD), through which we can obtain a single-crystalline, 1D, TiO_2 columns [1]. Due to the 1-Dimensional transport of the electron, height of the TiO_2 column effect the power conversion efficiency. Optimum column height is required for high efficiency, tall enough to propagate through most of the perovskite layer, but small enough to prevent electron-hole recombination. The focus of this work is to study the effect of height of these nanostructures, ranging from a flat ETL to roughly 1.5µm, on the power conversion efficiency. This comparison offers insight in determining the optimum column dimensions for high perovskite solar cell power conversion efficiency using ACVD.

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7MS.12

Controlling the Structure and Morphology of Functional Nanoporous Films Fabricated by Direct Deposition of Nanoparticles from Liquid Flame Spray (LFS). JYRKI M. MÄKELÄ, Janne Haapanen, Paxton Juuti, Miika Sorvali, Markus Nikka, Elham Baniadam, *Tampere University of Technology, Tampere, Finland*

Nanoparticles can be used as building blocks to fabricate larger entities of material, such as highly porous thin films and other types of deposits, which maintain high surface area of nanoparticles and typically possess the exquisite nanostructure, have high purity, tailored properties, controlled composition, degree of oxidation and particle size. Nanoporous thin films are used in gas sensing, energy storage, catalysis, pharmaceutics, biotechnology, etc. Also bulk and roll-to-roll material surface modification has been performed using porous nanoparticle thin films, resulting in superhydrophobic, superhydrophilic, anti-icing, anti-fogging, and antibacterial properties for the material.

We define Liquid Flame Spray (LFS) as one type of flame spray pyrolysis techniques to generate aerosol nanoparticles, based on combining a spray of liquid precursor droplets and a flame where the precursor evaporates, reacts and nucleates into nanoparticulate form. LFS, in particular, operates using hydrogen and oxygen as the combustion gas and oxidizing gas, respectively. The most common nanoparticle materials are noble metals, metal oxides and their mixtures, with nanoparticle size varying within the range 2-200 nm.

Recently LFS has been applied to several types of functional coatings by depositing the nanoparticles directly from the LFS flame to the substrate. Practical applications are numerous, but unfortunately the resistance of the nanoparticle film against wear is still relatively poor, for the time being. We present studies on solutions to strengthen the structure of these porous nanoparticle layers either as in situ process during the deposition or as post-treatment after the deposition. We have considered e.g. adding of binders, sintering, compression, and modifying of nanoparticle composition, to fix nanoparticles in place, still without losing the nanostructure and superior functionality.

7TT.1

Modelling Biomass Burning Plumes: The Impacts of Dilution, Chemistry, and Coagulation on the Size Distribution and Resulting Direct and Indirect Effects. ANNA HODSHIRE, Qijing Bian, Shantanu Jathar, Sonia Kreidenweis, Jeffrey R. Pierce, *Colorado State University*

Biomass burning is an important source of carbonaceous species to the atmosphere, with significant implications for air quality, climate, and human health. The direct and indirect radiative impacts of these particles depend on the size, composition, and amount of these particles in the atmosphere; hence, we need to understand biomass burning particle evolution in the atmosphere. Fires emit both primary organic aerosol (POA) and organic vapors of varying volatility that depend on the fuel and burning conditions. These particles and vapors evolve in the atmosphere due to chemistry and dilution. Many of the emitted vapors can undergo oxidation to become lower-volatility products that can then contribute to SOA production; some of the POA may be semivolatile and evaporate upon dilution; and some of the POA evaporation products may then oxidize to form lower-volatility products that can again participate in SOA production. The net production/loss of biomass burning organic aerosol depends both on chemistry and dilution in the plumes (Bian et al., 2017). Further, particles in the plume undergo coagulation, which reduces particle number and shifts the size distribution towards larger sizes. Coagulation, evaporation, and SOA production each depend, in part, on fire size and ambient conditions such as the atmospheric stability conditions (Bian et al., 2017; Sakamoto et al., 2016).

In this study, we use an expanding Lagrangian box model to simulate biomass burning plumes as they disperse and chemically and physically evolve. We simulate small to large fire sizes with areas between 1×10^{-4} and 1×10^{2} km^2, different stability conditions, and different background aerosol concentrations. For each fire/meteorological/background case, we perform sensitivity tests of each available combination between coagulation on/off and chemistry on/off to determine the role of coagulation, chemistry, and dilution on the evolution of the aerosol size distribution in biomass burning plumes. Finally, we calculate the efficiencies of the particles in each case to impact aerosol direct and indirect effects and determine the role of coagulation, chemistry, and dilution on direct and indirect effects.

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7TT.2

Spatial and Temporal Characteristics of Taklimakan Desert Dust and Its Air Quality Influence Using the WRF/CMAQ Model System. WENYE DENG, Jiaerheng Ahati, Xue Qiao, Xinjie Yuan, Kui Deng, Jing He, Weiyan Lin, Jing Yang, Jie Zhu, Weixin Du, Hongliang Zhang, *Xinjiang Academy of Environmental Protection Science*

Taklimakan Desert is surrounded with Tianshan, Kunlun and Altun Mountains, most of the desert dust is deposited in the Tarim Basin, and has serious impact on the air quality of near regions. In recent years, the ambient particulate matter (PM) concentrations in the cities in the Tarim Basin are exceeding the Ambient air quality standards of China, especially Hotan and Kashgar. . In this paper, the spatial and temporal distribution, production and deposition, and regional transport of desert dust aerosol over Tarim Basin in 2015 were quantified using the Weather Research and Forecasting model with the Community Multiscale Air Quality (WRF-CMAQ) model system. Combined with observation data, the simulation results show that the dust production was largest in spring, relatively small in summer and autumn, and reached its minimum value in winter, the highest annual dust deposition and ambient PM10 and PM2.5 concentration were appeared in Hotan and Kashgar. It is suggested that the spatial distribution and temporal variation in dust deposition and ambient PM10 and PM2.5 are closely related to the different underlying surfaces characteristics and meteorological conditions, wind speed, wind direction and precipitation. This is the first time that the WRF-CMAQ model system was used in the Tarim Basin with Taklimakan Desert dust emission, and the results are publicly available for future of the ecological environment protection and human health studies.

7TT.3

The Impact of Wet Deposition on Long-Range Aerosol Transport Arriving at the Maldives. JUTTA KESTI, John Backman, Eija Asmi, Ewan O'Connor, Orjan Gustafsson, Krishnakant Budhavant, *Finnish Meteorological Institute*

Wet deposition is a process where raindrops remove aerosol particles from the atmosphere. Precipitation intensity, aerosol particle size and other microphysical properties are all factors that affect the efficiency of wet deposition. This process is important but still poorly described in atmospheric models (Liu et al. 2012).

Precipitation is an important climate variable in the Maldives. During summer, the Maldives is under the influence of the Indian monsoon, which brings warm and moist marine air consisting mostly of natural aerosols from the Indian Ocean. During winter, which is the dry season, the air masses at the Maldives mainly travel from the Indian subcontinent and thus bring polluted air.

To study the effect of precipitation on long-range transported aerosol particles in the Maldives, we used two different data sets measured at the Maldives Climate Observatory of Hanimaadhoo (MCOH), one of the Atmospheric Brown Cloud (ABC) observatories (Ramana and Ramanathan, 2006). The first measurements were conducted during 2004–2008 using a Scanning Mobility Particle Sizer (SMPS.) The second measurement period was during 2014–2017, using a Differential Mobility Particle Sizer (DMPS). In addition, we collected the meteorological observation data measured at MCOH for these periods and calculated hourly back trajectories and cumulative rainfall along the trajectory for the measurement periods using HYSPLIT 4.9 model (Draxler and Hess, 1998). The meteorological data providing wind fields and precipitation for the back-trajectory model was the GDAS 1^{o} dataset from National Center for Atmospheric Research.

The results reveal different particle size distribution shapes depending on the source region of aerosol particles; the highest concentrations were observed in outflow from India and the Indo-Gangetic plain. The particle size distributions were also affected by the precipitation intensity en route to the measurement site. The median particle number concentration during the dry season in the first measurement period 2004–2008 was 624 1/cm3 and during monsoon season 178 1/cm3. For the second measurement period, during 2014–2017, the numbers were 1647 1/cm3 for dry season and 408 1/cm3 for monsoon season.

We also studied the change in the aerosol particle size distribution shape compared to different amounts of rainfall by using the cumulative rainfall from the model and in-situ measurements with the SMPS and DMPS. The analysis was divided to cover different source regions and seasons. Impact of precipitation on size distribution shape in the tropics for different aerosol types was then elucidated and compared with previous studies made in other locations (eg. Tunved et al., 2013).

We gratefully acknowledge the staff working at the Climate Observatory of Hanimaadhoo for maintenance of the measurements.

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7TT.4

Comparison of PM-Bound Polycyclic Aromatic Hydrocarbons and Nitropolycyclic Aromatic Hydrocarbons in Urban Air in the WHO's Western Pacific Regions. KAZUICHI HAYAKAWA, Ning Tang, Edward Nagato, *Kanazawa University*

The combustion of fossil fuels and biomass produces many kinds of air pollutants such as carbon dioxide, sulfur oxides, nitrogen oxides, polycyclic aromatic hydrocarbons (PAHs) and nitropolycyclic aromatic hydrocarbons (NPAHs). Large fractions of PAHs and NPAHs are found in airborne particulate matter (PM), especially fine particulate matter (PM2.5) which have a diameter no more than 2.5µm. Among these compounds, the International Agency for Research on Cancer (IARC) has classified benzo[a]pyrene (BaP) as a Group 1 compound (carcinogenic to humans), while dibenz[a,h]anthracene, 6-nitrochrysene and 1-nitropyrene (1-NP) are classified as Group 2A compounds (probably carcinogenic to humans). Moreover, 1,3-, 1,6-, 1,8-dinitropyrenes and 1-NP show strong direct-acting mutagenicity, and several PAHs and NPAHs show endocrine-disrupting and reactive oxygen species-producing activities. Recently, outdoor air pollution, including PM, has been classified into Group 1 by the IARC.

In this report, total suspended particulate matter was collected during the summer and winter seasons over two decades, in urban areas of more than 15 cities in the WHO's Western Pacific Regions and South-East Asia. PAHs, including pyrene (Pyr) and benzo[a]pyrene, were determined using high-performance liquid chromatography (HPLC) with fluorescence detection and NPAHs, including 1-nitropyrene (1-NP), were determined using HPLC with chemiluminescence detection. The concentration ratio of 1-NP to Pyr ([1-NP]/[Pyr]), which increases with an increase in combustion temperature, was used as a source marker for all cities.

In the Western Pacific Regions, Chinese and Russian cities showed much higher PAH and NPAH concentrations than Japanese and Korean cities. Chinese cities showed significant differences by season (Winter > Summer) and latitude (North > South). The smaller [1-NP]/[Pyr] ratios in northern and central Chinese cities suggested that the major contributors were winter coal heating or biomass burning, while the larger [1-NP]/[Pyr] ratio in south Chinese cities suggested that the major contributor was automobiles. In South-East Asia, Vietnamese and Thai cities showed relatively high PAH and NPAH concentrations. The [1-NP]/[Pyr] ratio was smaller in the wet season but larger in the dry season, suggesting that the major contributors are automobiles (motor bikes) during the wet season and slash-and-burn agriculture in the dry season, respectively. Atmospheric BaP levels in several cities in the regions were still much higher than the standards of the WHO (0.12 ng m-3) and the EU and China (1 ng m-3). Recent regional air quality has changed dramatically from the point of view of PM-bound PAHs and NPAHs.

7TT.5

Seasonal Variations of Mass Concentration and Chemical Composition of Fine Particulate Matter in a High-Elevation Subtropical Forest in East Asia – Impact of Anthropogenic and Biogenic Emissions. CELINE SIU LAN LEE, Charles C.K. Chou, Chien-Cheng Jung, Joe Hing Cho Cheung, Chao-Yang Tsai, *RCEC, Academia Sinica, Taiwan, R.O.C.*

The aim of this study was to characterize the fine particulate matter ($PM_{2.5}$) in a subtropical forest in East Asia under the influences of anthropogenic and biogenic sources and a complex topographic setting. A one-year measurement campaign was conducted in Xitou forest in central Taiwan to measure the mass concentrations of $PM_{2.5}$ and its components, including ionic (Ca^{2+}, Na^+, NH_4^+, K^+, Mg_2^+, Cl^-, NO_3^- and SO_4^{2-}) and carbonaceous (OC and EC) species. The aerosol chemical composition exhibited distinct seasonal variation. Non-sea-salt sulfate (nss-sulfate) constituted the major component of $PM_{2.5}$, followed by NH_4^+ and NO_3^- during winter, summer and autumn, while nss-SO_4^{2-} and NO_3^- contributed in similar mass fraction to $PM_{2.5}$ in spring season. The results showed that $(NH_4)_2SO_4$ was preferably formed, but a larger fraction of NH_4NO_3 was formed due to existence of strong NO_x sources in spring, which could be originated from local traffic exhaust or industrial sources. Higher secondary organic carbon was observed in summer, due to the enhanced photo-oxidation of biogenic precursors during summertime. Significant amount of K^+ was present which could be attributed to biomass burnings of straws and/or municipal waste incineration. The transport of pollutants from the urban sources was found to be critically driven by the mountain-valley circulation, where polluted air mass was uplifted and transported by the northwesterly winds (valley breezes) during the daytime, and relatively clean air mass was transported by the southeasterly winds (mountain breezes) during the nighttime. The diurnal variations of O_3 and SO_2 coincided with each other, suggesting that the pollutants are aged which were transported from distant sources, whereas CO and NO_x were shown to be under the influences of both local and regional emission sources. The sulfur oxidation ratio (SOR) for $PM_{2.5}$ measured in this study (0.878-0.952) was notably higher compared to that obtained in other urban sites (e.g. 0.12–0.39 in Beijing, 0.19 in Tianjin, and 0.22-0.62 in Italy). It is suggested that the aqueous-phase oxidation of SO_2 could be strongly enhanced under high RH condition (average RH of 87.1-92.1% for different seasons) of subtropical climate at the study site to form sulfate and hence attributed to the exceptionally high sulfur oxidation state. The nitrogen oxidation ratio (NOR) observed in this study (0.058-0.481) was also found to be higher than that observed in other urban sites (e.g. 0.04-0.08 in Beijing, 0.19 in Tianjin and 0.01-0.08 in Italy), indicating significant amount of NO_2 is converted to NO_3^-. This study exemplified the significant impact of anthropogenic pollutants from a megacity (with population over 2 million) and its suburbs, where intense industrial and biomass burning activities have occurred, on a high-elevation subtropical forest which itself is an important source of biogenic VOCs. The results showed that the interaction of both anthropogenic and biogenic pollutants have yielded significant amounts of secondary aerosols, mostly in the form of sulfate, followed by nitrate and other secondary organics products. The anthropogenic pollutants transported to the site have altered the atmospheric processing involved in particle formation in the forest, resulting in significant pollution which requires attention and further investigation.

7TT.6

Investigation of Spatial and Temporal Variations in Aerosol Mixing State Using a Particle-Resolved Regional Aerosol Model. JEFFREY H. CURTIS, Nicole Riemer, Matthew West, *University of Illinois at Urbana-Champaign*

The aerosol mixing state is critical for determining the microphysical interactions of particles with the large-scale atmospheric system, yet accurately capturing mixing state continues to be a major challenge for regional and global models. One of the aspects contributing to this challenge is that numerical models resort to simplified aerosol representations (modal or sectional) to reduce computational costs. These types of models greatly simplify the aerosol mixing state, and the assumptions made can result in errors in computed cloud and optical properties.

To quantify the importance of representing aerosol mixing state, the particle-resolved model PartMC-MOSAIC was coupled with the WRF model. The resulting model not only explicitly resolves and tracks the size and composition of individual particles as they undergo transformations by coagulation and condensation in the atmosphere, but also resolves the 3D spatial distribution of aerosols and trace gases, based on meteorological fields predicted by the WRF model. The novel computational methods developed for this purpose include a particle-resolved emission inventory and stochastic transport algorithms. Particle-resolved emissions are constructed using source apportionment in SMOKE. This source-oriented aerosol emission approach allows for different emission sectors to have varying aerosol composition rather than assuming all emissions of a given grid cell are internally mixed at the point of emission. Stochastic transport algorithms sample a small fraction of particles in each grid cell to be transported at each time step, allowing efficient advection and turbulent diffusion while maintaining numerical accuracy. With its fully-resolved mixing state representation, WRF-PartMC-MOSAIC allows for direct intermodel comparisons with aerosol schemes used in regional models (e.g., the sectional 4 or 8 bin MOSAIC), and climate models (e.g., MAM3/MAM4/MAM7).

We used WRF-PartMC-MOSAIC to simulate the spatial and temporal variations in aerosol composition over northern California during the CARES campaign in June 2010. Using the unique 3D particle-resolved aerosol data from the simulation, we directly compute 3D distributions of mixing state metrics and quantify the impact of mixing state on CCN and optical properties of the aerosol as it varies throughout the domain.

7TT.7

Assessment of the Possible Radioactive Particles Flux from the Surface in the Territory of the Russian Federation.

VILTORIA BYCHKOVA, Dmitriy Pripachkin, *IBRAE RAN, Russian Federation*

One of the possible ways of formation of radionuclide release in the atmosphere is the wind rise of radioactive aerosol particles from surfaces contaminated with radioactive substances. The report will describe software for assessing the possible impact of atmospheric emissions of radioactive substances on the environment – RELTRAN. The main objective of this method is to estimate the source of emissions in the atmosphere and to predict the radiation situation around nuclear object in the territory of Russian Federation. A quantitative characteristic of the rising by the wind dust (with the known radionuclide composition of previous depositions) is the flux of dust particles.

The study of wind soil erosion is at the crossroads of several disciplines: deflation theory of soil, soil science, atmospheric physics, the theory of turbulence in the lower atmosphere, etc. At the present time, to solve the problems of interaction atmosphere and land surface are widely used hydrodynamic atmospheric models (WRF-ARW, COSMO and etc.). Such models numerically resolve a wide range of meteorological processes and contain information on the characteristics of the underlying surface. However, it is not possible to use only hydrodynamic models within this task because of secondary dust formation are not described in the framework of numerical prognostic models. The wind-lifting and radioactive dust transfer processes require the creation of an additional physical description. Hydrodynamic models can be used in this work as a source of input data for the created RELTRAN software.

It is extremely important to determine the critical wind speed necessary for the beginning of the ascent of soil particles for creating a physical description of these processes. The method of determining the critical wind speed must take into account the soil properties. The upper soil layer humidity is a special characteristic, as it is subject to strong changes. In the event that the force of the air flow is sufficient to start the salting, the concentration of sand particles will be calculated at the salting level. The salting level defines as a function of the friction velocity [Buttner, 1978, Pomeroy et al., 1992].

The amount of the flow depends on the ratio of the actual speed to its critical value and on the thermo physical characteristics of soil. The magnitude of the flow will give an opportunity to estimate the scale of soil erosion. It is important to consider the number of potentially available dispersed soil particles for blowing. If the ability of the flow to carry suspended particles increases, the processes of formation the suspension are activated. Since the main source of the solid phase is a surface, the concentration of suspended particles will decrease with altitude in proportion to the rate of their settling.

For creating the RELTRAN software, optimal methods will be chosen for calculating the critical wind speed and the flow of sand particles for the territory of the Russian Federation.

7TT.8

Transboundary Transport of Anthropogenic Sulfur in PM2.5 at a Coastal Site in the Sea of Japan during 2013 to 2016.

YAYOI INOMATA, *Kanazawa University*

In Japan, which is located downwind of the prevailing winds drawn from the Asian continent, high concentrations of $PM_{2.5}$ were observed at several locations and times, the values exceeding the target value of environmental standard on daily average in Japan (35 maicrog m^{-3} per day). The sulfur isotopic ratio ($^{34}S/^{32}S$) is regarded as useful chemical tracers to investigate the source contributions of sulfate in aerosols and precipitation, because the values are different among the sources (1). In this study, daily observations of $^{34}S/^{32}S$ in $PM_{2.5}$ were carried out the Niigata-Maki site facing to the Sea of Japan during the intensive monitoring periods from 2013 to 2016.

Airborne particulate samples were collected at the National Niigata-Maki Acid Deposition Monitoring station (hereafter Niigata-Maki, 138.85°E, 37.81°N), which is located facing to the Sea of Japan. A high volume air sampler with $PM_{2.5}$ impactor (HVI2.5) was used to sampling. Intensive sampling was performed in four seasons from 2013 to 2016. The airborne particulate samples were collected over a 24 hr period. $PM_{2.5}$ samples were collected on a quartz fiber filter (2500 QAT-UP, Pall Science Co. Ltd.) after the coarse particles (diameter > 2.5 microm), which were collected on a separate quartz fiber filter (HV-SF, Pall Science Co. Ltd.). The samples were analyzed by stable isotope mass spectrometry (Delta Plus, Thermo Co. Ltd.). Canyon Diablo Troilite (CDT) was used as standard.

The $^{34}S/^{32}S_{nss}$ in $PM_{2.5}$ ranged from -0.1 to 6.7‰. It showed a seasonal variation with relatively higher values being observed in winter (2.3-6.7‰) compared with values in the other seasons (1.0-4.2‰ in spring, -0.1-4.5‰ in summer, 1.3-5.8‰ in autumn). These data were classified by using the air mass transport routes: directly transported air mass after leaving the Asian continent (TRB), the air mass transported over the Japanese islands after leaving the Asian continent (including domestic sources; DOM), and the air mass transported over the Pacific Ocean and the Japanese islands in summer (NPO). In 2016 summer, the air mass was transported over the Pacific Ocean before arriving at the Niigata-Maki monitoring station. The $^{34}S/^{32}S_{nss}$ in this period was 0.86±0.56‰, which are same level to the $^{34}S/^{32}S$ in oil. Considering that the dominant source of sulfate in Japan is oil combustion, these values suggest the domestic emission is dominant source to sulfate in summer. Furthermore, the $PM_{2.5}$ mass concentrations were relatively larger in summer compared with those in other season. The $^{34}S/^{32}S_{nss}$ suggest that the increase of aerosol mass concentrations is due to the mixing and growth by domestic precursor gases. In the air mass transported over the Sea of Japan after leaving the Asian continent and arrived to the Niigata-Maki, the $^{34}S/^{32}S_{nss}$ values for TRB (3.9±0.1‰) are higher than those for DOM (3.1±1.0‰). The $^{34}S/^{32}S_{nss}$ values for TRB were often observed in winter and close to the values in aerosol measured in northern China. It is also noted that the $^{34}S/^{32}S_{nss}$ values in TRB in winter are almost same from 2013 to 2016, although sulfate concentrations were decreased.

The lower $^{34}S/^{32}S\ _{nss}$ in the air mass transported over the Japanese islands arriving over the site (DOM) are resulting with mixing of the emissions from the Japanese islands and the transboundary transported SO_4^{2-} in $PM_{2.5}$. The relative contribution of transboundary transport component to sulfate in $PM_{2.5}$ was estimated by using the mass balance model. The relative contribution of transboundary component in TRB was 66±13%. The contribution from transboundary transport was large in winter. It is also noted that the relative contribution from DOM in summer are more than 60 %. These results suggest that $PM_{2.5}$ emitted from the Asian continent are modified during transboundary transport.

[1] Inomata et. al (2016) Sci. Total. Environ. 553, 617.

7TT.10

Aerosol Size Distributions in Lower Atmospheric Boundary Layer above Coal Strip Mine by Airborne Measurements.

JAN HOVORKA, Miroslav Klán, Milos Zapletal, Jana Esterlova, Jan Bendl, Filip Kobrzek, Petr Marecek, *Charles University in Prague*

Quantification of atmospheric aerosol emission by large-surface sources, like coal strip mines or agriculture fields, is usually calculated from emission factors. Since the factors significantly vary with the used technology and meteorology and orography of the mine or field play a major role in fugitive aerosol emissions, calculated emission rates significantly differ from real ones. To measure real aerosol emission rates from a large strip mine, eddy-covariant measurements by an unmanned airship carrying an aerodynamic particle sizer were conducted at heights 50-800m aloft a large lignite strip-mine in the Czech Republic in winter 2017/2018. There was a critical height at 350m above the mine bottom, approx. 120m above the edge of the mine, identified in the mine atmospheric boundary layer. Below the critical height, bimodal (0.6 and 6 µm) aerosol particle mass size distribution was recorded then suddenly changed to monomodal distribution at higher altitudes. Mass of submicron particles was constant (15µgm^{-3}) up-to the critical height while significantly dropped (5µgm^{-3}) above the height. In contrast, supermicron particle mass linearly decreased from 90% (max ~1 mgm^{-3}) to 25% (1 µgm^{-3}) at critical height and were constant at higher altitudes. Also, single technologies were detected as rather narrow columnar plumes up-to 80m below the critical height but the plumes were smeared and ceased at higher altitudes. This indicates rather low emission rates of atmospheric aerosol from the mine to neighboring environment under meteorology condition of the measurement.

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7TT.11

A Near-Global Analysis of In-Situ Profiles of Seasalt Aerosol. STEVEN HOWELL, Steffen Freitag, Nikolai Smirnow, *University of Hawaii*

Seasalt-derived particles are the largest contributor to aerosol mass on a global basis. Particularly in areas of the remote ocean, they are important contributors to light scattering and cloud droplet nuclei. Vertically-resolved atmospheric concentrations of sea-spray aerosol over the open ocean are sparse and are not well represented in chemical transport models. We have analyzed particle size distribution data from 14 NASA and NSF-sponsored airborne projects to assemble a collection of latitude-, longitude-, altitude-, and time-referenced SSA size distributions stretching over 20 years and including most of the world's ocean basins. Seasalt particle size distributions are determined with a variety of aerodynamic and optical instruments, including thermal treatment to drive off volatile materials. Where possible, they are referenced to chemical measurements and are generally correct to within 30%. Inlet corrections have been made, but only particles <10µm are considered. We show that chemical transport models can have large, systematic errors in both mixed layer SSA and the efficiency with which they are transported higher in the boundary layer and the free troposphere.

7TT.12

The Topography Contribution to the Influence of the Atmospheric Boundary Layer at High Altitude Stations. Martine Collaud Coen, Elisabeth Andrews, Dominique Ruffieux, FRANCISCO NAVAS-GUZMÁN, *Federal Office of Meteorology and Climatology*

High altitude stations are often emphasized as free tropospheric measuring sites but they remain influenced by atmospheric boundary layer (ABL) air masses due to convective transport processes. In this study, a topography analysis is performed allowing calculation of a newly defined index called ABL-TopoIndex. The ABL-TopoIndex is constructed in order to correlate with the ABL influence at the high altitude stations and long-term aerosol time series are used to assess its validity. Other important parameters influencing the aerosol load such as the wind, the soil state and the synoptic weather conditions were not taken into account.

We analysed 43 high altitude stations representative of 5 continents. The topography was taken from GTopo30. The ABL-TopoIndex relies on the criteria that the ABL influence will be low if 1) the station is one of the highest points in the mountainous massif, 2) there is a large altitude difference between the station and the valleys, plateaus or the average domain elevation, 3) the slopes around the station are steep, and 4) the «drainage basin» for air convection is small. These principles are implemented by the calculation of 5 parameters involving the hypsometric curve, the steepness of the slopes around the station and the drainage basin for convection. The geometrical mean of these five parameters is the ABL-TopoIndex and allows ranking of the stations as a function of the ABL influence due to convection.

The first observation is that all stations on volcanic islands (in this study) have very low ABL-TopoIndex (i.e., low BL influence), whereas the stations in the Himalaya and the Tibetan plateau have high ABL-TopoIndex. Mount Pico in the Azores and the Teide Observatory in Izãna rank as the stations with the lowest ABL influence because both islands comprise the highest summit in the archipelago and both stations are just below the summits. In contrast, PYR lies at the foot of Mount Everest and at the confluence of several valleys leading to a high ABL-TopoIndex. Mount Moussala, Bulgaria, Mount Helmo, Greece and Mount Washington Observatory, USA are stations situated at the top of their mountainous ranges, leading to ABL-TopoIndex similar to the volcanic islands.

Statistically significant correlations between the ABL-TopoIndex and the aerosol parameters measured at 28 high altitude sites allow validation of the methodological approach. The greatest correlations are found with the minima of the aerosol parameters that represent the most likely FT air masses. The maxima of aerosol parameters are more representative of the intensity of aerosol sources and of advection of air masses with high aerosol concentrations. There are also strong anticorrelations between the slope local steepness and the particle number concentration, suggesting that new particle formation could be largely influenced by this topographical parameter. The amplitude of the diurnal cycle of the absorption coefficient is also correlated with the ABL-TopoIndex and is, thus, likely to be representative of ABL influence. The strength of the diurnal cycles of the scattering coefficient and the number concentration are, however, mostly explained by the latitude of the station, leading to the conclusion that the insolation drives the aerosol diurnal cycle.

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All station managers having shared aerosol datasets to validate the ABL-TopoIndex are associated as co-authors and gratefully acknowledged.

7TT.13

Airborne Investigation of the Vertical Layering and Transport Processes of Aerosol Particles in the Marine Boundary Layer and the Free Troposphere over the Atlantic Ocean. BIRGIT WEHNER, Silvia Henning, Felix Lauermann, Janine Lueckerath, Greg Roberts, Kai-Erik Szodry, Holger Siebert, *Leibniz-Institute for Tropospheric Research*

Persistent low-level stratocumulus (Sc) clouds are widespread over the globe and cover on average about 20% of the Earth's surface and play an important role due to their influence on the planetary albedo. The Sc-topped boundary layer (STBL) is usually separated from the free troposphere (FT) by a thin layer characterized by strong gradients in thermodynamic and dynamic properties called entrainment interfacial layer (EIL). Closely connected to the stratification of the cloudy marine boundary layer is the spatial distribution of aerosol particles. Aerosol particles strongly interact with clouds, serving on the one hand side as cloud condensation nuclei (CCN). On the other hand, clouds are known as aerosol sources, due to new particle formation in their outflow or entrainment regions. These processes may have significant influences on both, particle and droplet number concentrations in the STBL. Furthermore, long-range transport of aerosol plays a significant role for the local balance. Due to the different sources and sinks of aerosol particles, the spatial aerosol distribution in marine areas is often characterized by complex layering closely linked to the boundary layer structure.

One main focus of this study is to improve the knowledge of sources and exchange processes of aerosol particles in the marine boundary layer. Therefore the measurement campaign “Azores stratoCumulus measurements Of Radiation, turbulEnce and aeroSols“ (ACORES) was conducted in order to have a detailed study of the stratification and layering of the marine boundary layer in terms of clouds and aerosol. ACORES took place in July 2017 on the Azores, an archipelago in the northeastern Atlantic Ocean located about 1200 km west of Portugal (39° N, 28° W). While being a remote place and having negligible influences of local anthropogenic sources, the Azores are considered being representative for the undisturbed North-East Atlantic, making it an ideal location for this study.

During the ACORES experiment airborne measurements were performed using the helicopter-borne ACTOS and SMART-HELIOS payloads which sampled almost from sea level up to 2200 m in the vicinity of Graciosa. The measurements were completed by continuous ground-based observations at sea level and in the free troposphere being the topic of a separate presentation.

For the period between July 3rd and July 22nd 2017, datasets from 17 research flights with ACTOS and SMART-HELIOS are available. The helicopter-borne payload ACTOS measured meteorological parameters with high temporal resolution, such as 3D-wind vector, temperature, and absolute humidity, but also aerosol particle number size distribution and total number concentrations of aerosol particles Np and CCN. A new pyrano- and pyrgeometer combination provides up- and downward radiation observations in the terrestrial and solar band. Furthermore, cloud droplet number concentrations, liquid water content and droplet size distributions are available.

A typical measurement flight comprises of a vertical profile up to 2000 m or higher at the begin of the flight, horizontal legs at various height levels in order to obtain robust statistics of quantities such as number size distributions and series of vertical profiles around a layer of interest, so called dolphin-flight patterns.

Number size distributions at different height levels are similar in shape: most of them consist of two modes being the typical structure for marine aerosol. However, the ratio between number concentrations of these modes varied mainly due to air mass origin. The vertical transport of aerosol particles between marine boundary layer and free troposphere will be investigated in more detail and will be subject of this presentation.

Vertical flights through the EIL show frequently enhanced particle number concentrations above the cloud layer indicating new particle formation. This process and the potential vertical transport of these newly formed particles will be investigated in this contribution.

7TT.14

Mobile Aerosol Measurement in Areas Around Coal-Fired Power Plants. SUJI KANG, Sungnam Chun, Gayoung Lee, Jinpyo Hong, *Korea Electric Power Corporation Research Institute, Korea*

Air pollution research and reports have been limited in south Korea, especially in Chung-nam Province located with many coal-fired power plants(18,050MW) with respect aerosol particle number and mass concentration and Chemical compositions.

This study aims to identify the characteristics of Fine Particulate Matters So that we utilized "KEPRI Mobile Lab" to measure, for 15 days (Jan 25 ~ Feb 9) at city of Boryeong
KEPRI Mobile Lab consisted of portable aerosol instruments to measure particle number concentration (1nm ~ 20 um), particle mass concentration (PM1.0, PM2.5), organic and element carbon, cation and anion concentration (PM1.0, PM2.5), Various gaseous measurement (VOCs, NOx, SOx and so on) and meteorological measuring instruments all situated on the back seat of 3.5-ton

Although the Measurement campaign was 15 days long, but it provided preliminary information about aerosol concentrations over areas mainly affected by Coal Combustion Gas. We should consider that the presented concentrations reflect on Vehicle and Ship Flue gas.

In this study, we expect to results shows that dramatic increase in the concentration of submicron particle concentrations (PM1.0) is observed because of northwester wind and long-range transport of air pollutants. The diurnal concentration has different peak characterization as time has gone (AM, PM). the results of the m/z 44(CCO+) and OA(organic aerosol) ratio using HR-ToF-AMS means OOA ratio is changed depends of wind directions.

7TT.15

The Sahara Desert Dust Contribution in the Central Amazonia Determined with in situ Measurements in the ATTO Tower and in the ZF2 Reserve and Remote Sensing Use.

RAYNER SANTOS, Paulo Artaxo, *National Institute of Research of the Amazon*

During the wet season, the Amazon receives intense dust emissions from the Sahara desert, which is the largest source of dust in the atmosphere, contributing to changes in climate and atmospheric chemistry at regional and global scales. Sporadically, this dust is accompanied by aerosol of biomass burning from the Sahel region. The Amazon region receives this dust through transatlantic transport, which acts in the long term as a valuable fertilizer in this ecosystem, providing essential nutrients to the forest. This work aims to quantify the aerosols transported to the Amazon from the North of Africa by the trade winds and to investigate the different compositions of the aerosols from continuous and long term measures in three sites in the Central Amazon, in a region of forest to north of the city of Manaus-AM. For the first time, from an extensive and diverse database it was possible to determine the elemental concentration of dust aerosols from the Sahara desert and Black Carbon (BC) of the Sahel, using the proton induction technique as well as X-ray fluorescence by dispersive energy (PIXE and EDXRF) applied to the filters obtained in a region of forest (ZF2), with validation from values present in the atmospheric column using data obtained from two AERONET Network Solar Photometers in the central region of Amazonia, as well as we measured the presence of the aerosols sampled from the influence on absorption and scattering. Products obtained by the NASA-Giovanni system, which provides access to a wide range of remote sensing data from NASA and other data sets, which associated with HYSPLIT transport modeling, provide a source-receiver relationship of the measured aerosols. It was identified that the presence of coarse particulate material is predominant between the second fortnight of January and the month of May, presenting a mean volumetric radius ranging from 1.30 µm to 8.71 µm, and contributes up to 78% of the Optical Depth of Aerosol (AOD 500 nm). The highest prevalence of dust aerosols occurred during this same period, with a concentration of 204,09 ± 604,09 ng/m3, and from 141 pairs of filters, 60 dust-intensive events were identified between 2008 and 2015, representing 85% of all identified dust. The BC has a lower presence in this period and has a concentration of 160.12 ± 158.14 ng/m3. The Ångström parameter was adjusted for the aerosol samples in the Amazon, showing, for dust, Angstrom values of spreading ≤ 1,11 and absorption ≥ 0,87. The relationship between backtrajector analysis and satellite products obtained from the MODIS Terra sensor showed that the origin of air masses coming from regions with high AOD in the Sahara and Sahel region contributed to ZF2. From these results we can conclude that the highest frequency of dust deposition during the wet season occurs between mid-January and May and its dry deposition represents 6.09% of the total aerosol mass measured in the period, and this deposition strongly impacts the coefficients of absorption and scattering of radiation.

8AC.1

Formula vs. Structure: Impacts of Isomers on Interpretation, Calibration, and Parameterization of Atmospheric Mass Spectrometric Data. GABRIEL ISAACMAN-VANWERTZ, Bernard Aumont, Manjula Canagaratna, Paola Massoli, John Nowak, Jordan Krechmer, Rachel O'Brien, Jesse Kroll, Douglas Worsnop, *Virginia Tech*

Recent advances in field-deployable mass spectrometry of gas- and particle-phase organic compounds have provided unprecedented characterization of atmospheric mixtures. However, while organic carbon across the entire range of atmospheric properties has become measurable by current state-of-the-art tools, many of these instruments identify analytes only by elemental formula with little or no structural information. The appearance of different isomers as the same chemical species (i.e. ion) may critically impact source apportionment, understanding of chemical processes, and instrument calibration. Furthermore, a substantial body of work has generated and utilized empirical parameterizations of molecular properties (e.g. volatility and reactivity) based on elemental formulas, despite these properties having strong structural dependencies. Consequently, it is possible the presence of isomers in ambient samples is a major source of uncertainty in data interpretation due to the lack of structural information provided by many instruments. However, the extent to which (unmeasured) isomers impact current understanding is not well known since no comprehensive effort has been made to catalog the importance of isomers in the atmosphere. We capitalize on a diverse set of published and new isomer-resolved measurements (gas chromatography, liquid chromatography, ion mobility) to answer the fundamental question: “How prevalent are isomers in the atmosphere, and what does this mean for our data?”. We find that molecular formulas typically represent several, and in some cases up to 10, isomers. Calibration and interpretation of gas-phase mass spectrometer data from a suite of biogenic oxidation experiments will be discussed in this context, and atmospherically-relevant structures generated by the GECKO-A model will provide estimates of the uncertainty isomers may introduce into current parametrizations.

8AC.2

Molecular Markers and Thermal Decomposition of Biogenic Secondary Organic Aerosol: Insight from Lab and Field Observations by Thermal Desorption – Gas Chromatography – Mass Spectrometry. MICHAEL WALKER, Riley Martell, Audrey Dang, Raul Martinez, David Hagan, Thomas Berkemeier, Masayuki Takeuchi, Gamze Eris, Nga Lee Ng, Brent Williams, *Washington University in St. Louis*

Secondary organic aerosol (SOA) constitutes a large fraction of global submicron aerosol. The composition of SOA is highly complex, consisting of thousands of different molecules that vary with both the source and atmospheric processing of the particles. Advances in mass spectrometry (MS) techniques have greatly increased our understanding of SOA composition. For molecular detection, most MS methods for SOA analysis either utilize chemical derivatization to alter SOA molecules to forms more amenable to gas chromatography (GC) separation, or rely on chemical ionization to select specific classes of molecules for detection. For both molecular-level analysis and bulk chemical analysis, MS techniques often rely on thermal desorption to introduce the collected aerosol. Several studies have demonstrated that thermal desorption techniques can thermally decompose samples such that the detected molecules are not necessarily the original SOA molecules. Stark et al. demonstrated that measured chemical formulas from chemical ionization mass spectrometry (CIMS) techniques cannot adequately predict the aerosol volatility (Stark et al., 2017). Additionally, during the initial thermal desorption step of a thermal desorption aerosol gas chromatograph (TAG), small, highly volatile fragments are produced from both organic and inorganic species (Williams et al., 2016). Measuring these fragment species enables the classification of decomposition products, which are not retained on the GC column.

Within the TAG family of instruments, the Volatility and Polarity Separator (VAPS) utilizes a thermal desorption step, followed by a modified two-dimensional GC technique coupled with a high-resolution time-of-flight mass spectrometer (Martinez et al., 2016). The VAPS inlet and newly incorporated miniature-GCs have several programmable temperature regions, which give unprecedented control to study the thermal decomposition of SOA.

Molecular markers and thermal decomposition products were recently studied through VAPS measurements as part of a larger study on the oxidation of biogenic volatile organic compounds (BVOCs) at the Georgia Tech Environmental Chamber. Specific molecular markers were determined for a range of SOA sources, but larger thermal decomposition fragments were most abundant from particulate organonitrate compounds that result from the NO3 oxidation of BVOCs, which have typically been identified with CIMS or LC-MS techniques (Ng et al. 2017). Despite the loss of direct information on the original SOA molecules, decomposition serves as a “thermal derivatization” process, in which the resulting distinct molecular fragments are more amenable to detection and can serve as decomposition tracers. In combination with additional oxidation experiments using a Potential Aerosol Mass (PAM) oxidation flowtube reactor, the identification of these decomposition tracers has led to new insights into field measurements by the VAPS and TAG systems from field measurements during the Southern Oxidant and Aerosol Study (SOAS), the St. Louis Air Quality Regional Study (SLAQRS), and a more-recent campaign at the Jefferson Street site in Atlanta.

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8AC.3

Making Quantitative Measurements in Environmental Chamber Studies of VOC Oxidation and SOA Formation: Evaluating and Accounting for Potential Sources of Error. JULIA BAKKER-ARKEMA, Paul Ziemann, *University of Colorado*

Controlled environmental chamber studies are important for determining atmospheric reaction mechanisms and identifying and quantifying gas and aerosol products formed in the oxidation of volatile organic compounds (VOCs). Such information is necessary for developing detailed chemical models for use in predicting the atmospheric fate of VOCs and also secondary organic aerosol (SOA) formation. However, complete analyses of atmospheric reactions, including both gas and particle phase product yields, branching ratios, and uncertainties, are difficult to achieve. When conducting laboratory chamber experiments, care must be taken to account for all the potential sources of error. For this work, we developed and evaluated a systematic approach for minimizing uncertainties by quantifying the gas- and particle-phase products of the oxidation of terminal alkenes by hydroxyl radicals in the presence of NO. Based on the results, we propose standard methods of accurately measuring chamber volume, adding precursors to the chamber, collecting gas- and particle-phase samples, and accounting for losses of vapors and particles to the chamber walls. We also investigated the generation of authentic standards with carefully calibrated mass measurements and corrections for solvent mass contributions. Particle-phase products were analyzed in real time with a thermal desorption particle beam mass spectrometer, and off-line by collection onto filters and subsequent analysis of functional groups by derivatization-spectrophotometric methods developed in our lab. Derivatized products were also separated by liquid chromatography for molecular quantitation by UV absorbance and identification using chemical ionization-ion trap mass spectrometry. Gas phase aldehydes were analyzed off-line by collection on a 5-channel denuder and subsequent analysis by gas chromatography, or by collection onto DNPH-coated cartridges and subsequent analysis by liquid chromatography. We demonstrate that when the proposed steps are taken to reduce the inherent uncertainties associated with environmental chamber experiments, we can comprehensively and accurately analyze the composition of complex mixtures of organic particles and gases formed in laboratory chamber studies.

8AC.4

Probing the Molecular Composition of Model Systems and Secondary Organic Aerosol during Evaporation. DAVID BELL, Veronika Pospisilova, Amelie Bertrand, Houssni Lamkaddam, Chuan Ping Lee, Ruby Marten, Jay G. Slowik, Andre S.H. Prévôt, Urs Baltensperger, Imad El Haddad, Josef Dommen, *Paul Scherrer Institute*

Secondary organic aerosol (SOA) makes up a significant fraction of the fine particulate matter in the atmosphere. Because of their prevalence in the atmosphere organic aerosol has a significant impact on human health and the earth's climate. Therefore, an accurate assessment of the time scale of the aerosol lifecycle is needed to evaluate its impact on the environment. One constraint on the aerosol lifecycle is its volatility. If a particle rapidly evaporates then the impact on the environment will be correspondingly short. However, if organic aerosol consists mainly of low-volatility components, it will not readily evaporate and will be long-lived in the atmosphere, undergo long range transport, and grow large enough to act as cloud condensation nuclei.

Extractive electrospray ionization time-of-flight mass spectrometry (EESI-TOF) is a soft ionization technique and makes it possible to determine the molecular composition of aerosols without fragmentation. Here, we will use EESI-TOF to follow the change in composition of a variety of aerosols during the process of iso-thermal evaporation. We will demonstrate that it is possible to separate changes from wall-losses versus evaporative losses. This technique will be expanded to probe the composition dependent evaporation of ideal multi-component systems and will be compared to their expected volatility. Finally, this method will be applied to complex SOA systems (α-pinene SOA and toluene SOA) generated in atmospheric simulation chambers. Here, we will discuss how the composition of SOA changes as a function of evaporation and aging.

8AC.5

Gas-to-Particle Partitioning of Major Oxidation Products from Monoterpenes and Real Plant Emissions as Measured by Three Novel Aerosol Chemical Characterization Techniques. Georgios Gkatzelis, THORSTEN HOHAUS, Ralf Tillmann, Iulia Gensch, Markus Mueller, Philipp Eichler, Xu Kang-Ming, Patrick Schlag, Sebastian H. Schmitt, Yu Zhujun, Rupert Holzinger, Armin Wisthaler, Astrid Kiendler-Scharr, *Forschungszentrum Juelich GmbH, Germany*

Secondary organic aerosol (SOA), formed through the oxidation of volatile organic compounds in the atmosphere, play a key role in climate change and air quality. Due to thousands of individual compounds involved in SOA formation, the chemical characterization of organic aerosols (OA) remains a huge analytical challenge. In this framework, a comparison of three different aerosol chemical characterization techniques has been performed. The aerosol collection module (ACM) (Hohaus et al., 2010), the chemical analysis of aerosol online (CHARON) (Eichler et al., 2015) and the collection thermal desorption unit (TD) (Holzinger et al., 2010) are different inlets connected to a Proton-Transfer-Reaction Time-of-Flight Mass Spectrometer (PTR-ToF-MS). These techniques were deployed in a set of chamber experiments at the atmosphere simulation chamber SAPHIR to investigate the composition of fresh and aged biogenic SOA from monoterpenes and real plant emissions. Furthermore, the partitioning of major biogenic oxidation products between the gas- and particle-phase was investigated.

Despite significant differences in the aerosol collection and desorption methods of the PTR-based techniques, the determined chemical composition was comparable, with the same major contributing ions found by all instruments. These ions could be attributed to known products expected from the oxidation of the examined monoterpenes. Differences in total mass recovery between the instruments were found to result predominately from differences in the electric field strength (V cm^{-1}) to buffer gas density (molecules cm^{-3}) (E/N) ratio in the drift-tube reaction ionization chambers of the chemical ionization instruments and from dissimilarities in the collection/desorption of aerosols.

Gas-to-particle partitioning values were determined based on the saturation mass concentration (C*) of the individual ions. Theoretical calculations based on the molecular structure of the compounds showed, within the uncertainties ranges, good agreement with the experimental C* for most semi-volatile organic compounds, while intermediate-volatility organic compounds deviated up to a factor of 300. These major differences point towards (i) possible interferences by thermal and ionic fragmentation of higher molecular weight compounds, produced by accretion and oligomerization reactions that show up at m/z’s detected by the instruments, as well as (ii) kinetic influences in the distribution between gas- and particle-phase with condensation to the particle-phase and irreversible uptake.

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8AC.6

Real-time Measurements of Gas/Particle Partitioning of Semivolatile Organic Compounds into Different Probe Particles in a Teflon Chamber. XIAOXI LIU, Douglas Day, Jordan Krechmer, Paul Ziemann, Jose-Luis Jimenez, *University of Colorado Boulder*

The partitioning of semivolatile organic compounds (SVOCs) into and out of particles plays an essential role in secondary organic aerosol (SOA) formation and evolution. Most atmospheric models treat gas/particle partitioning as an equilibrium between bulk gas and particle phases, despite potential kinetic limitations and differences in thermodynamics as a function of SOA and pre-existing OA composition. This study directly measures the partitioning of oxidized compounds in a Teflon chamber in the presence of single-component seeds of different phases and polarities, including oleic acid, squalane, dioctyl sebacate, pentaethylene glycol, dry/wet ammonium sulfate, dry/wet sucrose, and α-pinene SOA from ozonolysis. The oxidized compounds are generated by a 10 s OH oxidation burst of a series of alkanols under high NO conditions. A chemical ionization mass spectrometer (CIMS) was used to measure the decay of gas-phase organic nitrates, which reflects uptake by particles and chamber walls. We observed clear changes in equilibrium timescales with varying seed concentrations and in equilibrium gas-phase concentrations across different seeds. In general, the gas evolution can be reproduced by a kinetic box model that considers partitioning and evaporation to and from particles and chamber walls. The accommodation coefficient (~1) and saturation mass concentration of each compound in the presence of each seed are estimated using the model. The changes in particle size distributions and composition monitored by a scanning mobility particle sizer (SMPS) and a high-resolution time-of-flight aerosol mass spectrometer (HR-ToF-AMS) are investigated to probe the SOA formation and evaporation. The observed SOA mass enhancements are highest with α-pinene SOA, and lowest with wet ammonium sulfate and sucrose. SOA activity coefficients (γ) were estimated for each seed with two independent methods, from equilibrium gas-phase concentrations and from SMPS-measured SOA evaporation rates. Lower γ is found when SOA and the seed have similar polarities, indicating favorable interactions. In addition, α-pinene SOA does not appear to have a diffusive limitation to the uptake of SVOCs, since it behaves like a liquid even under dry conditions. This work investigates the applicability of partitioning theory to these systems and derives the relevant quantitative parameters that were previously uncertain and rarely measured.

8AC.7

Development of a Method for the Measurement of the Henry's Law Constant Distribution of Atmospheric Organic Aerosol. AIKATERINI LIANGOU, Kerrigan Cain, Petro Uruci, Antonios Tasoglou, Spyros Pandis, *University of Patras, Patras, Greece*

The Henry's law constant of organic aerosol (OA) components and their precursors determines their partitioning between the gas and aqueous-phases. It determines their dry deposition velocity, their wet deposition rates, and to a large extent their potential for significant aqueous-phase chemical transformations. The corresponding constants for specific atmospheric organic compounds vary from 10^{-4} to 10^{10} M atm^{-1}. There is very little information about the distribution of Henry's law constants for ambient OA and this creates significant uncertainty in the predictions of CTMs simulating semi-volatile OA.

In this study, an experimental method for the measurement of the Henry's law constant distribution of atmospheric OA is developed. The method relies on the separation of the OA components based on their volatility and then the measurement of the water solubility distribution of each fraction. The separation by volatility is performed using a thermodenuder (TD) and the volatility distribution is estimated using a TD aerosol dynamics model. The measurement of the solubility distribution is based on the extraction of the water soluble organic carbon from each sample using different amounts of water. The solubility distribution range can be further extended with cloud condensation nuclei (CCN) measurements of both the total OA and the different volatility fractions. The synthesis of the measurements results in the estimation of the Henry's law constant distribution of each volatility bin in the Volatility Basis Set framework.

The method was tested by measuring the Henry's law constant distribution of the products of the dark ozonolysis of a-pinene in a smog chamber. The results indicate a wide distribution of properties that can be now used in chemical transport models to improve the description of the removal of the corresponding compounds.

8AC.8

Laboratory Evaluation of Organic Aerosol Chemical Composition Measurements Obtained from High-Resolution Mass Spectrometers with Different Soft Ionization Schemes. JORDAN KRECHMER, Andrew Lambe, Felipe Lopez-Hilfiker, John Jayne, Douglas Worsnop, Manjula Canagaratna, *Aerodyne Research, Inc.*

Atmospheric organic aerosols remain an important topic of study because of their impacts on human health and climate. Historically, our community has lacked aerosol measurement techniques that are can measure a high mass fraction of organic aerosols with high chemical resolution at high time resolution. In attempt to achieve these goals, several techniques have recently been developed that combine soft-ionization and high-resolution time-of-flight mass spectrometry. Here, we discuss applications of a Filter Inlet for Gases and AEROsols coupled to a chemical-ionization mass spectrometer (FIGAERO-CIMS), a heated desorption inlet tube interfaced to a Vocus Proton Transfer Reaction Mass Spectrometer (PTRMS), and extractive electrospray ionization with mass spectrometry (EESI). We obtain simultaneous FIGAERO-CIMS, PTR-MS and EESI-MS measurements of secondary organic aerosol generated in an oxidation flow reactor. We examine the influence of thermal decomposition, chemical fragmentation, and ionization selectivity on FIGAERO-CIMS, PTRMS and EESI-MS measurements. Additional information obtained from the FIGAERO thermograms is assessed. We compare the on-line measurements with off-line electrospray ionization ion mobility mass spectrometry (IMS-MS) analysis, which allows for increased molecular-level identification via isobaric and isomeric separation and collisionally-induced dissociation. The fraction of organic mass characterized by these techniques is evaluated by comparison with organic mass concentrations obtained with an aerosol mass spectrometer.

8AC.9

Use of Continuous Measurements of the Growth Rate of Particles Inside Captive Aerosol Chambers to Study the Properties and Sources of the Species Responsible for Their Growth. DON COLLINS, Cassandra Milan, Jordan McCormick, Sean Kinahan, Joshua Santarpia, James Flynn, Matthew H. Erickson, Robert Griffin, Henry Wallace, Alexander Bui, *Texas A&M University*

Two Captive Aerosol Growth and Evolution (CAGE) chambers were operated in a clearing in a state forest north of Houston, TX to study the condensational growth rate of particles exposed to ambient levels of trace gases and solar radiation. The site is impacted by pollution from Houston and the surrounding region and by isoprene and monoterpene emissions from the surrounding forest. The chambers are roughly cubic meter cylinders constructed mostly of highly light transmitting FEP Teflon and surrounded by UV transmitting acrylic such that the solar spectral intensity inside approaches that outside. Efficient exchange of water vapor and trace gases across a sheet of gas-permeable expanded PTFE membrane that seals one end of the chamber maintains near-ambient gas composition inside. Monodisperse ammonium sulfate particles were intermittently injected and their size tracked over periods of several hours. By staggering the size of the injected particles new modes were added as soon as the existing mode(s) became difficult to track. The result is an almost continuous dataset of particle growth rate recorded over a two-month period in late summer and early fall. Complementary measurements of spectral solar intensity and of the concentrations of organic and inorganic trace gases were used with a simple box model to attribute observed particle growth to responsible precursor and oxidant gases. Among the salient findings from the study are i) growth rate was only weakly dependent upon particle size and ii) only minimal particle shrinkage or evaporation was observed. Nitrate radical chemistry was active in the early evening, resulting in a study average growth rate from 8:00 – 9:00 p.m. of 5.8 nm/hr that was comparable to the peak daytime growth rate of 6.1 nm/hr from 9:00 – 10:00 a.m.

8AE.1

Characterization of the Potential Exposure of Vulnerable Communities to Traffic-related Air Pollutants in Urban Microenvironments. CHEOL H. JEONG, James M. Johnson, Cuilian Fang, Peter Murphy, Jon M. Wang, Kerolyn Shairsingh, Barbara Lachapelle, Christopher Morgan, Greg J. Evans, *SOCAAR, University of Toronto*

Epidemiological and toxicological studies have demonstrated that exposure to traffic-related air pollutants (TRAP) has a wide range of adverse health impacts, especially in more susceptible population groups like children. The concentrations of TRAP (e.g. ultrafine particles (UFP), black carbon (BC), and nitrogen oxides (NOx)) vary spatially with distance from roadways due to rapid changes in atmospheric processes and meteorological conditions. In a busy downtown area, concentrations of TRAP show more localized gradients due to frequent vehicle congestions, the urban street canyon effect, and compact land and building development. For children, school location is an important determinant of exposure to traffic-related air pollution since students attending schools close to major roads can be exposed to elevated TRAP. High spatial and temporal resolution measurements are needed to evaluate personal exposure to air pollution levels in various urban environments.

To better characterize spatial gradients of TRAP in an urban environment, mobile measurements were made around busy downtown streets, urban recreational areas, and school areas in Toronto, Canada. A suite of portable devices was carried along timed and planned routes through traffic dense downtown streets up to a few kilometers, while a mobile laboratory van equipped with laboratory scale instruments was used to investigate potential exposure to TRAP around school sites. In addition to the mobile monitoring, TRAP measurements at multiple fixed monitoring stations across Toronto were made to validate the mobile monitoring data and increase the spatial and temporal resolution. The proximity of schools to major roads was determined and the relationship between TRAP concentrations measured at the school sites and the school proximity to major roads was evaluated.

Strong spatial variation of BC and UFP were found within a few kilometers in the compact downtown area and levels increased within deep urban canyons caused by tall office towers. Preliminary results indicated that BC and UFP levels increased at schools as their distance from major roadways decreased from 800 m to 100 m. UFP and BC levels at schools as far as 350 m from major highways were still higher than at a fixed site in downtown Toronto. Development of micro land use regression models for UFP and BC using the mobile and stationary monitoring data will be discussed.

8AE.2

Fine Paritculate and Black Carbon Exposure for Users of a Bus Rapid Transit System: Role of Vehicle Age and Impact of Fleet Renewal. RICARDO MORALES BETANCOURT, Boris Galvis, Juan Manuel Rincón, Maria Alejandra Rincón, Yadert Contreras Barbosa, *Universidad de los Andes*

This research documents the extremely high exposure concentration to fine aerosol particles ($PM_{2.5}$), black carbon (BC), and carbon monoxide, CO, experienced by users of one of the world largest Bus Rapid Transit (BRT) systems, located in Bogota, Colombia. Extensive sampling of the system was performed over a span of 12 months covering all branches of the system and a significant fraction of the system stations. Sampling of PM, BC, and CO was performed on-line using portable devices at a 10 second resolution. The particle size distribution was determined using an optical particle sizer. Gravimetric samples were collected to determine average trip concentration. Physical activity was determined in real time using portable accelerometers. Average ratio of in-bus to background concentration was 9:1 for $PM_{2.5}$ and 5:1 for CO. Nearly 50% of in-bus fine particulate mass was found to be BC, suggesting most of the particulate pollution in the system comes from diesel combustion. In-bus exposure level is shown to be strongly correlated with vehicle emission standard and vehicle kilometers traveled. The contribution of a typical round trip in the BRT system was estimated to account for 60% of PM2.5 daily dose, and between 75% to 85% of BC daily dose. Exposure levels where twice as large for passengers inside BRT buses with Euro II and III emission standard compared to those in Euro IV or V vehicles. The significantly lower exposure to $PM_{2.5}$, BC, and CO observed for commuters in bus models with stricter emissions standards suggests that a renewal of the older portion of the fleet could have a disproportionately large effect on reducing population exposure to air pollutants. This large benefit is shown to be only possible in cities with moderate air pollution levels and a marked gradient of in-bus to background pollution levels. The results of our observations are likely to be relevant to many cities given the rapidly growing number of BRT systems being implemented in large urban centers around the globe.

8AE.3

Comparing Real-Time In-Cabin/Outdoor Particulate and CO Concentrations during Car Commutes along Freeway and Non-Freeway Roads, and Whilst Idling at Traffic Lights, in Saint Louis, MO. ANNA LEAVEY, Nathan Reed, Sameer Patel, Kevin Bradley, Pramod Kulkarni, Pratim Biswas, *Washington University in St Louis*

Exposure to urban air pollution is associated with detrimental health effects and increased morbidity and mortality[1]. In developed countries, traffic emissions contribute 25-40% to urban air pollution, and as much as 90% for specific pollutants such as carbon monoxide (CO) and ultrafine particles[2]. An individual may therefore receive a disproportionately high amount of their daily exposure whilst traveling along roads. In the US, 91% of commuters travel to and from work by car. In fact, Missouri car drivers have experienced a 37% increase in the vehicle miles traveled between 1990 and 2013; this is set to increase another 20% by 2030[3,4].

Real-time simultaneous particulate ($PM_{2.5}$, lung-deposited surface area (SA), PNC) and gaseous (CO) concentrations were collected outside and inside of an on-road car operating with either windows open or closed, fan on or AC on, during 54 real commutes to and from Washington University in St. Louis. Commutes were then split into: 1) 16 non-freeway (NFW) roads (N = 249); 2) 2 freeways (FW) (N = 84); 3) idling/accelerating from traffic lights (N= 242); 4) following a bus or other high-polluter. The influence of road-type, traffic density, vehicle speed, lane position, and lead vehicle on both outdoor and in-cabin pollution was examined using linear mixed-effects models and ANOVA regression. The aim was to identify ways to minimize in-cabin exposure without modifying the outdoor pollutant environment.

Higher outdoor pollutant concentrations were measured on FWs compared to NFWs (b = 0.39-0.55; p-value <0.01) due to higher densities of vehicles and trucks, although correlations were complicated by vehicle speed. Higher $PM_{2.5}$ concentrations were observed whilst traveling on the slow and middle lanes of a FW compared to the fast lane (b = 1.35; b = 1.42; p-values = <0.01), and whilst following a truck (b = 0.034). Decreasing outdoor PNC and lung-deposited SA concentrations were observed on NFWs with decreasing traffic densities, and results suggest a small percentage of “gross-polluters” may be largely responsible for the measured CO concentrations. Outdoor concentrations were the strongest predictors of cabin concentrations (adj-R^2 values of 0.30-0.95), especially on FWs, although having the windows closed or the AC on produced a protective effect, reducing the infiltration of outdoor particles into the vehicle thus reducing commuter exposure. The ventilation variable influenced PNC the most (R^2 = 0.06), and CO the least.

Significantly higher outdoor pollutant concentrations were measured during acceleration compared to idling (>8%-17%), but may depend on the vehicle’s position in the idling line, for example, lower outdoor PNC were observed when the vehicle was accelerating from the front of the line versus further back (b = -0.220, p-value = 0.09), supporting transport policies that reduce wait times at traffic lights. Finally, elevated pollutant concentrations were measured whilst following school buses. Transport planners and commuters may mitigate exposures by adjusting traffic-light times, routes traveled, avoiding heavy polluters, and applying a dynamic approach to ventilation choice.

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8AE.4

Exploring the Socio-Economic Inequalities in the Exposure to Air Pollutants during Commuting by Different Travel Modes. IOAR RIVAS, Prashant Kumar, Alex Hagen-Zanker, *University of Surrey*

Commuters usually remain in close proximity to the main source of air pollution in urban areas: road traffic emissions (Dons et al., 2011). These emissions from combustion processes, mainly in a particulate form, are suspected to be particularly harmful (WHO, 2013). Previous studies suggest inequalities in exposure, with people residing in the most deprived areas generally experiencing higher concentrations of air pollutants (Fecht et al., 2015). The objective of this work is to determine differences between transport mode in the exposure during commuting to different fractions of Particulate Matter (PM), Black Carbon (BC) and ultrafine particle number concentrations (PNC) in London. Moreover, we investigated the determinants of the concentrations through linear regression models, as well as the presence of possible inequalities related to income deprivation. We monitored the previously mentioned pollutants in typical commutes from four London areas with different levels of income deprivation (G1 to G4, from most to least deprived) by car, underground and bus (the most popular transport modes) at three different times of the day (morning peak, afternoon off-peak and evening peak). The highest BC and PM concentrations were found in the G1 route while the highest PNC was observed in G3. G2 showed the lowest concentrations of all pollutants. We did not observe a direct relationship between income deprivation and pollutant concentrations, suggesting that differences between transport modes were more important. The underground showed the highest PM concentrations, followed by buses and, with much lower concentrations, cars. BC concentrations were also higher in buses than cars due to a higher infiltration of outside pollutants into bus. BC could not be measured in the underground due to interferences with iron in the measuring system. PNCs were highest in buses, closely followed by cars and lowest in underground due to the absence of combustion sources. Regression models indicated that the variation in the concentrations for each transport mode was mainly explained by wind speed or ambient concentrations (evaluated in separate models) and, to a lower degree, by route and period of the day. In multivariate models, wind speed was the common significant predictor for all pollutants in car and bus; and the only significant predictor for the different PM fractions. For the underground, wind speed was not a determinant. However, line and type of windows on the train explained 42% of the variation of PNC and 90% of all PM fractions. Statistics from Census data revealed that people from less deprived areas have a predominant use of car, and therefore receive the lowest doses (Respiratory Deposition Dose, RDD <1 $\mu g \cdot h^{-1}$) during commute while producing the largest emissions per commuter. Conversely, commuters residing at higher income deprivation areas have a major dependence on the bus, receiving higher exposures (RDD between 1.52-3.49 $\mu g \cdot h^{-1}$) while generating less emissions per person. This situation falls within the core principle of environmental justice as reviewed by Brulle and Pellow (2006). Therefore, there is a need to include the socioeconomic dimension in exposure assessment to account for the environmental injustice that may affect the exposure levels.

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8AE.5

Quantifying High-resolution Spatial Variations and Local Source Impacts of Urban Ultrafine Particle Exposure. PROVAT SAHA, Naomi Zimmerman, Luke Snell, Joshua Apte, Allen Robinson, Albert A. Presto, *Carnegie Mellon University*

To quantify the fine-scale spatial variations and local source impacts of urban ultrafine particles (UFP) exposure, we conducted systematic measurements of the concentration of UFP at thirty (30) sites in Pittsburgh, Pennsylvania. Sites were selected to span a range of urban land use attributes, including urban background, near-local and arterial roads, traffic-intersections, near-highway, urban street canyon, and restaurant density. 3-6 weeks of continuous measurements of particle number concentration were collected at each site using a rotating network of condensation particle counters (CPC). Other measurements included PM2.5, NO2, CO, O3, SO2, CO2, temperature and RH at each site.

Spatial variations in urban UFP concentrations varied by about a factor of three. Background and nucleating particle concentrations are relatively uniformly distributed while spatial variations are driven by local sources. Traffic is an important contributor to local spatial variations. Near arterial roads UFP concentrations are ~2 times than the regional background; in the urban street canyon and near-highway UFP concentrations are ~3 times higher. Other sources, such as restaurants and cooking emissions, are also important in certain micro-environments.

There are substantial diurnal and weekday/weekend variations in urban UFP concentrations. On a relative basis, there is stronger rush-hours traffic influence at high traffic sites compared to background sites, indicating the spatial pattern of UFP concentrations evolves over the course of the day. For example, the UFP concentrations on the weekday morning traffic-rush hours are 20-30% higher than daily-average near arterial roads and highway sites, whereas it is only 10% higher in the background sites.

Long-term particle size distribution measurements indicate that freshly nucleated particles only contributes ~10% of average UFP concentrations at urban background sites in Pittsburgh. Therefore, people with higher UFP exposure are exposed to more fresh particles emitted from local sources, which might have higher toxicity. More than 50% of Pittsburgh residents live near-local sources and are therefore exposed to elevated UFP concentrations. We are developing a land use regression (LUR) model for UFP concentrations to assess the population impacts and to explore the association between trends in UFP and other pollutants. The results from this study provide new insights into the extent of spatial variations and local source impacts of urban UFP exposure to improve air pollution policy and decision making.

8AE.6

The Fresh Air Wristband: Measuring Personal Environmental Exposures Using a Wearable Air Pollutant Monitor.

ELIZABETH LIN, Sarah Esenther, Fareeha Irfan, Massimiliano Mascelloni, Krystal Godri Pollitt, *University of Massachusetts Amherst*

Current personal air pollutant monitoring systems include backpacks containing hand-held air monitors and filters/pumps which are worn for several days. Given the size, weight and cost of these sampling systems, use with vulnerable populations (*i.e.*, pregnant women, infants) is not feasible. There has been limited development of analytical techniques to capture the cumulative exposure of an individuals to multiple air pollutants. New exposure assessment tools are required to better study longitudinal environmental exposures. We have developed the Fresh Air wristband to profile personal organic air pollutant exposures using a non-selective passive sampling technique. Pollutants are collected onto a sorbent bar housed within a silicone wristband. The sorbent bar is coated with a thin-film polymer substrate (polydimethylsiloxane) which accumulates non-polar air pollutants with a log K_{ow} ranging between 4 and 8. The wristband is worn by an individual for a multi-day period and then analysed using high resolution gas chromatography time-of-flight mass spectrometry with thermal desorption. With this personal exposure assessment tool, we can quantify the time-weighted averages of exposure to over 50 volatile and semi-volatile organic compounds during typical daily activities without impairing motion. We will present data on the functionality of the Fresh Air wristband as a non-selective passive air pollutant sampler. Application of this new personal exposure assessment tool in a cohort of 60 school-aged children residing in Springfield, MA will further be discussed. Improved assessment of exposure using the Fresh Air wristband across life stages (pregnancy, infancy, childhood) has the potential to produce a more comprehensive understanding of the air pollutants that mediate adverse health.

8AE.7

Evaluation of Portable Instruments for Measuring Nanoparticles Exposure and Respirator Performance under Simulated Workplace Conditions. ZIQING ZHUANG, Evanly Vo, Matthew Horvatin, *NIOSH*

Recent advances in aerosol instrument technology have made it possible to produce small, light, and portable format instruments for measuring aerosol particles, especially nanoparticles under laboratory conditions. Questions have emerged regarding the field use of portable instruments. These include: 1) how to wear these portable aerosol instruments while workers conduct their normal work without any interferences, 2) how to operate and perform across different body positions (bending, side-to-side reaching, and movement), and 3) how these instruments can withstand workplace environments. Thus, the aim of this study was to develop a new method of evaluation for portable instruments, including the handheld condensation particle counter (CPC), portable aerosol mobility spectrometer (PAMS), optical particle sizer (OPS), and NanoScan scanning mobility particle sizer (NanoScan SMPS) for measuring nanoparticles exposure and respirator performance under simulated workplace conditions.

The portable instruments were mounted to a tactical load bearing vest or backpack and carried on the back of the test subject while conducting simulated workplace activities. Simulated workplace protection factors (SWPFs) were measured using human subjects exposed to NaCl aerosols. Before beginning a SWPF test for a given respirator model, each of 10 subjects had to pass a quantitative fit test. Each SWPF test was performed using a protocol of five exercises for three minutes each: 1) normal breathing while standing, 2) deep breathing, 3) bending at the waist, 4) walking gently in place, and 5) a simulated laboratory-vessel cleaning motion. Two particle devices of each field portable instrument type and two SMPSs were used simultaneously to measure the upstream (outside the respirator) and downstream (inside the respirator) test aerosol. SWPF was then calculated as a ratio of the upstream and downstream particle concentrations. The results of the SWPF study show that geometric mean SWPF (GM-SWPF) was highest for the NanoScan OPS combined, followed by PAMS, and CPC.

This study demonstrated that NanoScan OPS, PAMS, and CPC could be used for measuring nanoparticle exposures under simulated workplace conditions. This study also provided the advantages and limitations of each individual portable instrument when 1) wearing it while workers conduct their normal work, 2) performing across different body positions (bending, side-to-side reaching, and movement), and 3) determining how each instrument can withstand workplace environments. Therefore, the results from this study could be used with appropriate caution, when selecting a suitable portable instrument for aerosol particle measurement and evaluation of respirator performance in nanotechnology workplaces.

8AE.8

Characterization and Quantification of Hexavalent Chromium and Other Air Toxic Metals in Communities Surrounding Metal Processing Facilities. EDWARD FORTNER, Paola Massoli, Tara Yacovitch, Scott Herndon, Andrey Khlystov, David Campbell, John Jayne, *Aerodyne Research, Inc.*

Hexavalent chromium is one of the seven hazardous air pollutants (HAPs) of primary importance to the U.S. EPA National Air Toxics Trends Stations (NATTS) program and it can be emitted into the atmosphere by facilities which conduct metal grinding, forging and plating operations if proper pollution control measures are not utilized. In March of 2018 the Aerodyne Mobile Laboratory (AML) conducted measurements of hexavalent chromium and other metals in the particle phase in an area in California focusing on the areas around businesses conducting these metal processing operations These facilities and neighborhoods have been studied previously with filter based measurements but this campaign was the first to conduct on-line fast time response (1 Hz) measurements of chromium in these areas that we are aware of.

The Aerodyne mobile lab contained a variety of fast time response instruments for the measurement of gas and particle phase species and features separate inlets for gas and particle phase species. Gas phase measurements included CO, CO_2, NO_2, NOx, O_3 and selected VOC's measured by proton transfer reaction mass spectrometry (PTR-MS). These gas phase species give useful insight regarding the chemical composition of the sampled air mass which can be related to sources. For the particulate chromium VI measurements key instrumentation included the Steam-Jet Aerosol Collector – Long Path Absorption Spectroscopy system (SJAC-LPAS) and the laser vaporization aerosol mass spectrometer (LV-AMS). The SJAC-LPAS conducted speciated measurements of Chromium VI and has a 15 second sampling time resolution but also has an 8 minute delay due to sample transfer from the point of collection to the optical cell. The LV-AMS detects chromium but is unable to determine the oxidation state., The unique attribute of the LV-AMS is that its fast time response (1 Hz) was used to locate chromium containing plumes which were then sampled with the SJAC-LPAS to speciate the chromium. Particle size information was also obtained with the LV-AMS and particle number concentration was determined with a condensation particle counter (CPC). Meteorological parameters of importance including wind direction are measured along with GPS coordinates to assist in plume mapping.

8AE.9

Detail Characterization of Aerosol Physical Properties of Mainstream and Sidestream Cigarette Smoke. TA-CHIH HSIAO, Ying-Jyun Chen, Hsiao-Chi Chuang, Chin-Sheng Tang, *National Central University*

Mainstream cigarette smoke is a major concern for smokers, and the sidestream cigarette smoke contribute to the neighboring people through passive smoking. Many studies have established mathematical models to predict the particle depositions in different regions of the respiratory tract. The particle size distribution (PSD), density, charging status and morphology are known as the important parameters affecting the deposition fraction. However, most of the studies solely address the importance of PSD. In this study, the aerosol physic properties of cigarette smoke particles are characterized and studied for the dose of respiratory deposition.

For conducting the well-controlled experiments, an automatic cigarette smoke generator(Smoking Machine) was designed and manufactured. It can host 16 cigarettes and control the individual ignition time. Following the Smoking Machine, an aerosol dilutor was used to avoid exceeding the upper detection limits of aerosol instruments and suppressed the particle coagulation for high-concentration cigarette smoke. The dilution factors are 1:200 and 1:80 for mainstream smoke and sidestream smoke respectively. The particle size distribution was measured by scanning mobility particle sizer (SMPS, TSI 3936). Aerotrak (TSI 9000) was used to measure the particle surface area concentration deposited in the alveolar region. Aethalometer (Magee AE31) and DustTrak (TSI 8530) were employed to measure the BC and PM2.5 mass concentrations respectively. In addition, the novel tandem DMA-AE31 system was established to provide the size selective BC and UVPM mass concentrations of cigarette smoke. Aerosol Electrometer (AE, TSI 3068B) was applied to determine the average electric charge of particles. At the same time, Aerosol Particle Mass Analyzer (APM, Kanomax 3601), the widely used real-time aerosol mass classification instrument, was used to tandem with DMA and SMPS (a.k.a. DMA-APM and APM-SMPS tandem systems) to estimate the effective density of mainstream and sidestream smokes in different size ranges. Some of these aerosol characteristics of cigarette smoke particles are first time being revealed and valuable for lung deposition and inhalation toxicity studies.

8AM.1

Developing Model Surrogates for Monoterpenes to Improve Predictions of Secondary Organic Aerosol. ISAAC AFREH, Bernard Aumont, Marie Camredon, Richard Valorso, Kelley Barsanti, *University of California, Riverside*

Global emissions of biogenic volatile organic compounds (BVOCs) are on the order of 1000 Tg carbon yr^{-1}. Monoterpenes ($C_{10}H_{16}$) account for approximately one-fifth of the total estimated BVOC emissions. Monoterpenes also represent a significant mass fraction of VOCs emitted during biomass burning, particularly from coniferous fuels. These atmospherically relevant monoterpenes exhibit large diversity in molecular structure. For example, in pine and spruce biomass burning samples, approximately thirty isomers were identified. Once emitted to the atmosphere, monoterpenes can impact climate and air quality through the production of secondary organic aerosol (SOA). The extent of SOA formation is dependent on the mass of the emitted compound, its atmospheric reactivity, and the volatility of oxidation and reaction products. To represent SOA formation in chemical transport models a gas-phase chemical mechanism is used to represent the reactivity of VOCs and subsequent oxidation product formation. To enhance computational efficiency, most gas-phase mechanisms adopt simplification strategies whereby individual VOCs are lumped into surrogate species, largely based on the reactivity of these compounds with hydroxyl radical. While such mechanisms are routinely used for modeling SOA, the lumping approaches have not been optimized to best represent the reactivity and properties of VOCs that serve as precursors to SOA. Monoterpenes are often represented by one model surrogate in gas-phase chemical mechanisms and SOA parameterizations used in chemical transport modeling, even though monoterpenes are known to have diverse chemical structures, different reaction rates with atmospheric oxidants (by orders of magnitude), and varied propensity for SOA formation.

In this work, optimization of the number and identities of monoterpene model surrogates was pursued by evaluating factors that influence SOA production including the reaction rates and products of monoterpenes with atmospheric oxidants, and the products and extents of SOA formation. GECKO-A, an explicit chemical mechanism generator and SOA model, was used to simulate SOA formation from ten individual monoterpenes under a range of NOx conditions, precursor concentrations, and particle loadings. The relative reactivity of the monoterpenes, the gas- and particle-phase products formed, and the rates and yields of SOA production were considered in optimizing the surrogates. Results to be presented include the SOA yields for each monoterpene under the different simulation conditions, the distribution of gas- and particle-phase species in the carbon oxidation state – volatility space, and the mass-based contributions of compounds to SOA as a function of number of carbons and functional groups. Further, the criteria for defining the optimum number of surrogates for monoterpenes will be presented. The GECKO-A based SOA formation analyses developed in this work form the basis for future work on optimization of model surrogates to better represent other classes of SOA precursors in gas-phase chemical mechanisms and SOA parameterizations used in chemical transport modeling. A broader consideration of the chemistry relevant for SOA formation and representation of that chemistry in chemical mechanisms will ultimately lead to more accurate predictions of the air quality and climate impacts of SOA.

8AM.2

Growth Kinetics and Size Distribution Evolution of Viscous Secondary Organic Aerosol. RAHUL ZAVERI, John Shilling, Alla Zelenyuk, Jiumeng Liu, David Bell, Emma L. D'Ambro, Cassandra Gaston, Joel A. Thornton, Alexander Laskin, Peng Lin, Jacqueline Wilson, Richard Easter, Jian Wang, Allan Bertram, Scot T. Martin, John Seinfeld, Douglas Worsnop, *Pacific Northwest National Laboratory*

Low bulk diffusivity inside viscous semisolid atmospheric secondary organic aerosol (SOA) can prolong equilibration timescale, but its broader impacts on aerosol growth and size distribution dynamics are poorly understood. We present here quantitative insights into the effects of bulk diffusivity on the growth and evaporation kinetics of SOA formed under dry conditions from photooxidation of isoprene in the presence of a bimodal aerosol consisting of Aitken (ammonium sulfate) and accumulation (isoprene or α-pinene SOA) mode particles. Aerosol composition measurements and evaporation kinetics indicate that isoprene SOA is composed of several semivolatile organic compounds (SVOCs), with some reversibly reacting to form oligomers. Model analysis shows that liquid-like bulk diffusivities can be used to fit the observed evaporation kinetics of accumulation mode particles, but fail to explain the growth kinetics of bimodal aerosol by significantly under-predicting the evolution of the Aitken mode. In contrast, the semisolid scenario successfully reproduces both evaporation and growth kinetics, with the interpretation that hindered partitioning of SVOCs into large viscous particles effectively promotes the growth of smaller particles that have shorter diffusion timescales. This effect has important implications for the growth of atmospheric ultrafine particles to climatically-active sizes.

8AM.3

A Finite-Element Method (FEM) Study on the Deposition of Non-spherical Graphite Particles in High Temperature Gas-cooled Reactor (HGTR). ZHU FANG, Yiyang Zhang, Mingzhe Wei, Xinxin Wu, *Tsinghua University*

In this study we discuss the deposition of non-spherical particles in cross-bundle flows. The background is the transport of graphite dust particles in the primary circuit of high-temperature gas-cooled reactors (HTGR). These highly non-spherical particles, coupling with fission products, partly deposit when flowing through the tube bundles of steam generator. In severe accident e.g. water ingress or loss-of-coolant, the deposited particles may re-suspend and contribute to the radiation source term. Therefore it is important to obtain a good estimation of deposition rate and distribution of graphite particles in HTGRs. The understanding of non-spherical particles deposition is limited by the lack of tool. Discrete element method (DEM) is more suitable for spherical and quasi-spherical particles. Molecular dynamics (MD) simulation is too expensive for micro-sized particles. Here we present a modified finite element method (FEM) study on the impact of micro-sized non-spherical particles. Our main effort is to include the effect of adhesion and damping. The adhesion force is derived from JKR model, correlated with contact area and then manually applied at the contact zone. The damping is incorporated through Rayleigh damping. First we validate the simulation results by comparing to Wall’s experiments. Then the method is extended to disk-like graphite particles. The critical capture velocities for different sized particles and different impacting angle are obtained. The results show the mass equivalent diameter is the dominant factor. The stable restitution coefficient increases with the decrease of particle size, while the critical velocity decreases rapidly. When the mass equivalent diameter remains constant, the restitution coefficient decreases with the lager sphericity. Then the particle impact model is incorporated to the LES modelling of particle-laden flow in tube bundles. The result shows that the deposition rate of small particles (<2 μm) is mainly controlled by the collision rate rather than sticky efficiency due to larger critical velocity. The turbulence and thermophoresis are the essential mechanisms. In contrast, the deposition rate of larger particles mainly depends on sticky efficiency. Thus the deposition rate first increases first and then decreases with the increase of the mass equivalent diameter. All those results can help to obtain a more credible estimation for deposition rate of the graphite particles in HGTRs.

8AM.4

Modelling the Evaporative Behaviour of Secondary Organic Aerosol Formed from α-pinene. YU MORINO, Kei Sato, Shantanu Jathar, Kiyoshi Tanabe, Satoshi Inomata, Yuji Fujitani, Christopher Cappa, *morino.yu@nies.go.jp*

Volatility determines the gas-particle partitioning of organic compounds, thus volatility is a key property to understanding the behaviour and to simulate concentrations of organic aerosol in the atmosphere (OA). Various studies had been conducted to experimentally measure and numerically simulate volatility distributions of OA, and over the last decade, it has been found that the evaporation of OA was slower than that expected by equilibrium models. It had been suggested that formation of low volatility compounds, such as oligomers, or particle phase diffusion could limit the evaporation of OA, though contributions of these factors still remain uncertain.

In this study, we experimentally investigated the volatility of secondary organic aerosol (SOA) from α-pinene ozonolysis by external dilution chamber experiments and chemical composition analysis. Volatility distributions were estimated from compositions observed by Proton Transfer Reaction Mass Spectrometry (PTR-MS) and Electrospray Ionisation Mass Spectrometry (ESI-MS). In addition, we conducted model simulations using the statistical oxidation model with processes of kinetic gas-particle partitioning, formation/dissociation between monomers and dimers, and particle-phase diffusion limitations.

Both experimental and modeling results showed that low volatility compounds had important contributions to SOA. The slow evaporation rates during the dilution experiment could be reproduced by the model either by assuming that the SOA was semi-solid (bulk diffusion coefficient of 10-15 cm2 s-1) or assuming that the oligomerization reactions resulted in high dimer formation rates and low dimer dissociation rates.

8AM.5

Causal Models as a Tool for Analyzing Dependence Structure of Variables in Combustion Aging Data. VILLE LEINONEN, Olli Sippula, Petri Tiitta, Ari Leskinen, Juha Karvanen, Annele Virtanen, Santtu Mikkonen, *University of Eastern Finland*

We investigated evolvement of small-scale wood combustion emission in environmental aging chamber. On-line measurements of aerosol size distribution and chemical composition and several gas concentrations from the chamber were performed using SMPS, AMS, PTR-MS and several gas analyzers. Total of five primary (POA) and secondary organic aerosol (SOA) factors from AMS data have been identified from OA mass spectra using PMF [1]. Both dark and UV induced aging were studied.

Evolution of emission in aging chambers has been studied by changing different chemical, physical and burning-device related factors that can have an effect on evolvement and SOA potential of emission. Many of these factors are dependent, so changing one of those factors can result in a change in other factors too. Therefore, taking into account the dependence structure of variables is necessary. Otherwise, intended univariate effect of factors are confounded by the changes of other factors, and improper analysis can lead to false conclusion of how intervening of factor changes variable of interest.

Aim of this study is to model evolution of emission in the aging chamber using multivariate statistical model. Furthermore, goal is to determine variables affecting each measured variable. Understanding the structures of impacts between different atmospheric variables is crucial when making decisions about constraints of different emission constituents.

Here we investigate applicability of causal modeling in case of analyzing complex environmental chamber data. We present preliminary results about using causal discovery algorithms and causal models.

Causal discovery algorithms search dependencies between variables by using either correlations observed in data, using fit of statistical model as a criterion, or both. The resulting causal structure is presented as a directed acyclic graph. Because dependencies found using causal discovery algorithms are based on data only, we evaluated meaningfulness of each dependency and removed known false dependencies from causal structure.

Using the obtained causal structure as a starting point, it is possible to estimate the causal relations between the variables and create a causal model. Causal model determines how each variable is influenced by other variables [2]. Model enables us to divide the effect of intervening of a factor to direct and indirect effect and thus make proper conclusions of causes of change in a variable of interest.

By using causal models, we were able to model evolvement of key gases such as NOx and ozone and size distribution and chemical composition of aerosols. We were also able to quantify the effects of components of POA and SOA to O/C-ratio of total organic aerosol. Finding emphasizes the potential of causal discovery algorithms to discover effects from multivariate data. In addition, causal models can estimate effect sizes. This is important when comparing importance of different variables to measured evolvement and comparing effect of intervening value of some variable to other variables.

In general, this study shows that causal models are useful when analyzing multivariate data, where multiple variables affect a variable of interest, and those effects are dependent. Model used in this study can be applied to different fuel types and to different environmental chambers. This enables rapid model development and gaining knowledge about the whole process occurring in the chamber. When the model is constructed, it can be used to predict how change in one emission component affects to others, especially the components of main interest: climate effects and toxicity. Adding new variables, including toxicity of emission is also possible and one of the main research objectives in the future.

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8AM.6

Monte Carlo Simulations of Particle Production and Processing: The Role of Evaporation and the Applied Nucleation Theories. GREGOR KOTALCZYK, Ivan Skenderovic, Frank Einar Kruis, *University Duisburg-Essen*

The correct prediction of the properties of produced (or processed) aerosol particles makes complex modelling approaches necessary. Many simultaneous processes, such as coagulation, nucleation, condensation and evaporation have to be considered in a population balance modelling (PBM) approach, which makes the solution of the corresponding equations difficult.

Many simplifications are therefore applied, commonly, the evaporation of newly formed particles is not considered. Such an approach is justified in the cases of a chemical decomposition of a chemical precursor (e.g. (Lindackers et al., 1997)), but it might lead to grave deviations in the cases of physically induced nucleation, like it is encountered in condensation-evaporation reactors, during laser-ablation, or in the process of spark or arc discharges.

We present a Monte Carlo (MC) method based on weighted simulation particles (Zhao et al., 2009) for the solution of the PBM equations, which describes all the processes mentioned above including the evaporation. The recently proposed stochastic methodology (Kotalczyk and Kruis, 2017) for coagulation and nucleation is thereby coupled to a deterministic simulation of the growth and evaporation equations by means of an operator splitting approach (Celnik et al., 2007).

Recent studies have shown that the incorporation of the evaporation leads to severe deviations from the simulations without the evaporation for certain metallic systems under isothermal conditions (Kotalczyk et al., 2017). In this study, similar findings are presented for Fe and Ag systems, under typical non-isothermal conditions, which are encountered during particle production processes.

It is found, that the inclusion of the evaporation processes is necessary for certain applied temperature profiles. The deviation of the evaporation containing results from the non-evaporation containing results are discussed in dependency of the applied temperature gradient.

We also discuss the role of the applied nucleation theory, several classical approaches (differing in several orders of magnitude for the nucleation rates, as described in (Girshick and Chiu, 1990)) are compared with each other. It is found, that under certain temperature profiles, the inclusion of the evaporation process is of more significance than the choice of the nucleation theory.

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8AM.7

Estimation of Nucleation and Condensation Rates From Size Distribution Measurements Using Statistical Inverse Methodology. MATTHEW OZON, Aku Seppänen, Anton Laakso, Jari Kaipio, Kari Lehtinen, *University of Eastern Finland*

Motivations

Aerosols play a key role in the global radiative balance of the earth. Their number concentration, size distribution (SD) and chemical composition affect their ability to scatter and absorb solar radiation as well as the formation, properties and lifetimes of clouds. The same properties determine how particles enter the human lung and cause various public health problems. To quantify these effects, we need to be able to determine the rates of the key microphysical processes, aerosol formation and growth, from measurements of aerosol SD evolution.

Methods

The estimation of nucleation rate and condensation rates still typically relies on rather simple visual analysis, regression methods or balance equations involving crude approximations. So far, e.g. determining both size and time dependence of condensation rates has been a challenge. In addition, the methods have not considered measurement uncertainty in a rigorous way. We propose an automated method based on the Kalman Filter (KF) — a very famous statistical, dynamical inversion method that is stable, minimizes the variance of the estimates and easy to implement. However, instead of using the KF only for filtering the SD, it is tweaked to also estimate the nucleation and condensation rates. This method requires no assumption of SD shape as it relies only on a physical evolution model — the aerosol General Dynamic Equation — and a measurement model — DMPS — that are both combined in the KF framework.

Results

As a proof of concept of our method and a test of its performance we analyze synthetic data — SD — that are generated by solving the GDE with a sectional method. We simulate eight days with four having a new particle formation event. The size spectrum ranges from an arbitrary critical cluster size of 2nm to 2µm. One single vapor is responsible for condensational growth. The simulated data are corrupted by additive and multiplicative noise in order to resemble actual measured data. The tests are conducted on two versions of the method: 1) estimation of two parameters, the nucleation rate and the vapor concentration — assuming a model for the size dependence of the condensation rates — and 2) estimation of the nucleation rate along with all the condensation rates without any insight of the theory. The results are really promising;the first derivation of the method is resilient to the data quality and allows to retrieve the nucleation coefficient used for the simulation, and the second variation of the method gives similarly good estimates for the nucleation rate and fair evaluations of the growth rates — even though the condensation rates suffer discrepancies for poor data quality.

8AM.8

Equilibration Timescale of Atmospheric Secondary Organic Aerosol Partitioning under a Wide Range of Temperature and Relative Humidity.

YING LI, Manabu Shiraiwa, *University of California Irvine*

Secondary organic aerosol (SOA) formed from partitioning of oxidation products of anthropogenic and biogenic volatile organic compounds (VOCs) accounts for a substantial portion of atmospheric particulate matter. Traditionally, SOA particles have been assumed to be homogeneous and well-mixed liquids and the VOCs oxidation products rapidly establish a gas-particle equilibrium partitioning. However, recent laboratory experiments as well as atmospheric measurements have demonstrated that SOA can occur in amorphous solid or semi-solid phase states, which may result in a kinetically-limited growth rather than the quasi-equilibrium growth. Simulations of the equilibration timescale (τ_{eq}) of SOA gas-particle partitioning under room temperature found τ_{eq} could be up to hours or days for organic aerosol associated with semi-solid particles (Shiraiwa & Seinfeld, 2012). It is important to further assess the temperature and relative humidity conditions under which such a dynamic formulation of SOA formation is required. This study applies a state-of-the-art kinetic flux model KM-GAP (Shiraiwa et al., 2012) to evaluate the timescale to achieve gas−particle equilibrium under a wide range of temperature and relative humidity. Effects of volatilities of condensing species, pre-existing particle sizes and number concentrations on τ_{eq} are also assessed. This study has implications in gas-particle interactions in the free and upper troposphere where particles may occur mainly as amorphous semi-solid or glassy phase states (Shiraiwa et al., 2017).

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8AM.9

Advancements in Aerosol Thermodynamics for Large-Scale Applications – Bridging the Gap between Structure and Volatility-Based Models. KYLE GORKOWSKI, Andreas Zuend, *McGill University*

The aerosol thermodynamics frameworks used in current chemical transport models (CTMs) do not explicitly account for non-ideality and liquid-liquid phase separation. These effects are arising from the molecular interactions and incomplete miscibility among organic and inorganic aerosol species. These processes are not accounted for due to three main reasons: (1) the necessity for computationally efficient frameworks, which entail some level of simplification, (2) a lack of model availability for the treatment of phase separation in the CTM context, and (3) limited molecular-level information about aerosol composition. We present work on improving the treatment of these effects in CTMs.

The Aerosol Inorganic—Organic Mixtures Functional groups Activity Coefficients (AIOMFAC) model is a structure-based activity model that explicitly incorporates solution non-ideality, including organic-inorganic interactions. The use of AIOMFAC in our improved phase equilibrium algorithm enables consideration of liquid-liquid phase separation in thermodynamic equilibrium calculations. Here we use this advanced thermodynamic treatment by AIOMFAC to assess the potential for improvements to existing two-product and 1-D volatility basis set approaches with regard to gas-particle partitioning under variable relative humidity (RH). We use an additional term to describe the RH-dependence in the widely used two-product and 1-D volatility basis set representations of aerosol mass concentration and gas-particle partitioning. As RH increases, the characteristic gas-liquid partitioning parameter, C*, of a component tends to decrease, driving additional organic mass from the gas phase to the particle phase. Depending on how liquid-liquid phase separation is treated in simplified models (i.e., complete inorganic-organic split, homogeneous single-phase, etc.), the resulting particulate mass will be either underestimated or overestimated in comparison to a more demanding calculation allowing for partial miscibility at equilibrium. In addition to building extensions to the currently used aerosol thermodynamic models, we have worked on increasing the computational speed of the AIOMFAC-based model. The model uses optimization to high precision as a default, so we performed a systematic assessment of the computational accuracy and speed of the AIOMFAC-based equilibrium model under various simplifying assumptions. We will discuss the challenges and feasibility of implementing an AIOMFAC-based thermodynamic module directly into a CTM.

8CB.1

Gasoline Aromatic and Oxygen Content Impact on Formation of Secondary Aerosols from a GDI Vehicle. PATRICK ROTH, Jiacheng Yang, Ayla Moretti, Thomas D. Durbin, David R. Cocker III, Akua Asa-Awuku, Georgios Karavalakis, *University of California, Riverside*

Gasoline powered motor vehicles have been identified as the dominant PM contributor (primarily in the form of SOA) surrounding heavily urbanized areas. Future scenarios indicate that the largest impact on premature mortality in California will be attributable to transportation emissions, particularly vehicular exhaust. Gasoline vehicles emit a variety of volatile organic compounds (VOCs), and deviating concentrations of NOx, CO, CO2, and PM. The PM that is emitted from gasoline vehicles is a complex mixture of black carbon (BC), organic aerosols (POA), and inorganic salts which varies with engine technology, age, and fuel used.

As of 2015, GDI engines accounted for approximately 45%, and 60% of the North American and European market respectively. PFI vehicles have significant advantages (low PM), but are expected to struggle meeting future legislation and fuel economy regulations. GDI engines, on the other hand, have improved fuel economy through an increased compression ratio and better air/fuel ratio accuracy. Another major driving force to differing emissions is variations in fuel content. Studies have shown that by varying ethanol and aromatic content, several regulated emissions also change. These differences can greatly affect both the tailpipe pollutant measurements and also the potential secondary aerosol formation from the exhaust.

For this study, eight gasoline fuels were blended to simulate high and low aromatic fuels (20% and 30% by volume) along with varying ethanol content (0 to 20% by volume). These fuels were tested with one MY-2017 GDI vehicle over a cold start LA92 driving cycle, in duplicate. The tailpipe emissions were measured to certification standards, while simultaneously injecting the tailpipe emissions into UCR’s 30m3 Mobile Atmospheric Chamber (MACh). The emissions were injected through the full driving cycle, and then subsequently aged for approximately eight hours. While the emissions were aging, the aerosol and gasses were monitored in real time with a host of gas phase and particle instruments. The presented work will explore the effects of low vs high aromatic fuel blends for E0, E10, E15, and E20 fuels, while also examining the differences in fuel blending techniques (match vs splash).

8CB.2

Effect of Fuel Properties on Diesel Engine Exhaust PM Physicochemical Characteristics. LI XINLING, *Shanghai Jiao Tong University*

Motor vehicles, especially diesel vehicles, became one of main sources of atmospheric PM2.5, therefore it is very important to control emission of diesel engines by building the inherent relationship between fuel properties and exhaust particle. In this paper, several fuels of different physicochemical characteristics available for compression ignition engine, were studied by using SMPS, HRTEM, TGA, Thermal Optical Carbon Analyzer and GCMS, and the effect of fuel properties, such as sulfur, aromatics, oxygen and other physical parameters on particle size distribution, nanostructure, oxidation reactivity and chemical components was analyzed. The work aims to build the inherent relationship between particle size distribution, nanostructure, oxidative activity and chemical components and provides a scientific basis for the controlling of the atmospheric PM2.5 derived from motor vehicle emissions.

8CB.3

Effect of Fuel Oxygen Content on Morphology and Nanostructure Characteristics of Diesel Particulate Matter. PUNEET VERMA, Mohammad Jafari, Edmund Pickering, Yi Guo, Svetlana Stevanovic, Richard Brown, Zoran Ristovski, *QUT, Australia*

There is an increased need for the adoption of oxygenated fuels such as biodiesel, alcohol fuels as an alternative to petroleum-based fuel first of all to reduce greenhouse gas emissions and to reduce dependencies on fossil fuels. To understand the soot formation and oxidation process, the morphology and nanostructural characteristics of diesel particulate matter for different fuels has to be investigated in a comprehensive manner. Literature has shown that biodiesel has lower tendency of producing soot emissions compared to petroleum diesel, thus can be a good alternative fuel to counter rising particulate emissions. To understand the effect of fuel oxygen content on morphology and nanostructure characteristics of diesel particulate matter, different fuels such as fatty acid based biodiesel, n-butanol and triacetin were tested in a diesel engine with various mixing proportions. The fuel blending was done in such a way that overall oxygen content of fuel was kept in range of 0 to 14.23% (wt.%). The diesel engine particles emissions were sampled from exhaust with the help of Nanometer Aerosol Sampler (NAS) and collected on 300 mesh holey carbon grids. The samples were then analysed with Transmission Electron Microscope (TEM) JEOL-2100 maybe put the model here) to acquire images of soot particles with low and high resolution. A MATLAB based image processing program was developed to characterise the different properties such as primary particle diameter, primary particle number density, fractal dimension, fringe length, fringe tortuosity and fringe separation distance. The change in the above properties as a function of fuel oxygen content will be presented. The notable finding of this investigations has been decrease in primary particle diameter and increase in fractal dimension with increase in fuel oxygen content.

8CB.4

Nanoparticle Emissions from a Gas Engine – Effects of Gas and Lubricant Oil Composition. MIA ISOTALO, Jenni Alanen, Joonas Vanhanen, Sampsa Martikainen, Hannu Vesala, Rasmus Pettinen, Sanna Saarikoski, Minna Aurela, Pauli Simonen, Mika Kettunen, Minna Väkevä, Hilkka Timonen, Kati Lehtoranta, Jorma Keskinen, Topi Rönkkö, *Tampere University of Technology*

Natural gas is a promising and clean energy source and its utilization is quickly increasing. The use of other gases, such as ethane and propane, may also increase in future energy production. Biogases solely or mixed with natural gas are becoming more and more relevant. To assure the sustainable development of societies, the usage of cleaner energy sources in the future is inevitable.

Although gas engines have been thought to be a good possibility to reduce atmospheric emissions, recent studies have shown that the natural gas combustion can emit large numbers of nanoparticles (Alanen et al., 2015). For that reason, the aim of this study was to examine the nanoparticle concentrations in the fresh emission of gas engine. Two lubricant oils with different sulphur and ash content were tested to investigate the influence of lubricant oil on concentrations of nanoparticles. The effect of gas composition to the amount of emitted exhaust particles was also one objective.

The measurements were conducted in laboratory using a gasoline engine of a passenger car that has been modified to run with used fuels (natural gas and propane) before the measurement campaign (Murtonen et al., 2016). Also two different engine driving modes were used.

In this study, two different dilution systems were used. A combination of a hot ejector and an ejector dilutor was used to study primary particle emission. In delayed primary particle emission measurements, the sample went through a porous tube diluter followed by a residence time chamber and an ejector dilutor. The volatility of the particles was studied using a thermodenuder or a catalytic stripper (Amanatidis et al., 2013). Particle number concentration was measured using several condensation particle counters (TSI Inc. and Airmodus Ltd.) with different cut-points (1.3, 3 nm, 4 nm and 10 nm) and particle size magnifier (Airmodus Ltd.). In addition, particle size distributions were measured using an SMPS (TSI Inc.) and a Nano-SMPS (TSI Inc.).

The sizes of observed particles were very small with both fuels. According to the preliminary results, in the fresh exhaust emission approximately 53 % of the all observed particles (total concentration) were in the size range of 1.3–3 nm and approximately 47 % in the size range of 3–10 nm, when natural gas was used and lubricant oil contained higher amount of sulphur. The use of lubricant oil with lower sulphur content caused significant reduction in total particle number concentration and the mean size of observed particles also decreased considerably. With this oil, approximately 79 % of the all observed particles were in the size range of 1.3–3 nm and 21 % in the size range of 3–10 nm. The contribution of particles over 10 nm in size were below 1 ‰ of the total concentration. For propane, the emissions of particles were extremely low.

The financial support from Tekes (NewGas project) and from industrial partners, Wärtsilä Finland Oy, Dinex-Ecocat Oy, Dekati Oy, Neste Oyj, Oilon Oy and Airmodus Oy, is gratefully acknowledged.

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8CB.5

Effect of High-Speed Driving Conditions on SOA Formation Potential from GDI Vehicle. NIINA KUITTINEN, Stephen Zimmerman, Weihan Peng, Cavan McCaffery, Patrick Roth, Pauli Simonen, Jorma Keskinen, Topi Rönkkö, Roya Bahreini, David R. Cocker III, Georgios Karavalakis, *Tampere University of Technology*

Aerosol particles from vehicle emissions are one the main contributors to impaired air quality and visibility in urban areas. It has been shown that, in many cases, the mass of secondary organic aerosol (SOA) formed as a result of photochemical oxidation of exhaust vapors in the atmosphere exceeds the emitted primary particulate matter. Traditionally, secondary aerosol formation potential has been studied using environmental chambers into which exhaust sample is collected throughout a transient driving cycle. Recently, some studies applying flow-through type oxidation reactors have indicated that SOA formation is highly dependent on vehicle driving condition. In these studies, well-established driving cycles such as the NEDC have been investigated. However, the ability of cycles like NEDC or the FTP to represent real-world driving conditions has been questioned, and some new driving cycles have been developed that better mimic the driving patterns in urban areas and freeways. In this study, the SOA formation potential of a modern GDI vehicle is examined over a variety of drive cycles representing different driving conditions.

Testing was conducted over duplicate cold-starts FTP, NEDC, and LA92 cycles and over duplicate hot-starts US06, Highway Fuel Economy Test (HWFET), and a set of cycles developed by the California Department of Transportation (Caltrans). The Caltrans cycles were developed to represent realistic driving conditions in California roads and characterized by high speeds (65 mph to 75 mph) and lower speeds (0 mph to 60 mph). Testing was performed on a GDI light-duty vehicle equipped with a wall-guided injection system and operating on typical California E10 fuel. Primary emissions measurements included gaseous pollutants, total and solid particle number, black carbon, and particle size distributions. The atmospheric aging of the emissions was studied using two parallel methods. TUT Secondary Aerosol Reactor (TSAR), a laminar oxidation flow reactor that allows real-time characterization of secondary aerosol formation, was applied for online measurements during the driving cycles. In addition, exhaust sample was injected to UC Riverside's Mobile Atmospheric Chamber (MaCh) to compare the average SOA forming potential over one completed cycle, as well as to gain in-depth information on the formation process. The secondary aerosol was characterized using scanning mobility particle sizer (SMPS), volatility DMA (VDMA), and aerosol particle mass analyzer (APM), combined with high resolution time-of-flight aerosol mass spectrometer (HR-ToF-AMS) for bulk chemical composition. For the real-time oxidation with the TSAR, an electrical low pressure impactor (ELPI+) and a mini aerosol mass spectrometer (mAMS) were applied to measure real-time secondary particle mass, as well as bulk chemical composition of the SOA, respectively. The observations made during this study underline the effects of varying driving patterns on the SOA formation from GDI vehicles and allow comparison of SOA results between an atmospheric chamber (batch testing) and an oxidation flow reactor (real-time testing).

8CB.6

Modeling Particle Emission Formation in Wildland Fires. ALEXANDER JOSEPHSON, Troy Holland, Rod Linn, *Los Alamos National Laboratory*

Presented is a surrogate model for predicting particle emission formation in wildland fires implemented in FIRETEC, a physics based CFD software designed for simulating the coupled behaviour of fire and the local atmospheric. This surrogate model was created using a physics-based detailed model previously published. The detailed model was used in fine-grid LES simulations to predict the formation of soot precursors and soot particles under a variety of circumstances. Results from these simulations were used to map input parameters to output data creating an array of correlations. It is these correlations that are the surrogate model.

The surrogate model can be used to predict a representative particle size distribution formed and released from the flame-zone of a wildfire along with total mass yields of 'black carbon'. It also predicts a mass yield of 'brown carbon' also released from the flame-zone. It is this 'brown carbon' that acts as soot precursors while in the flame; however, once released from the flame these species form a different kine of emission, thus the prediction of both 'black' and 'brown' carbon becomes invaluable to total wildfire emissions.

Presented is a synopsis of the detailed particle formation model along with some of the results of the fine-grid LES simulations. Also presented are details of the surrogate model, along with some preliminary results of its use in FIRETEC, as well as future usage and adaptation of this model.

8CB.7

Comparing On-Road and Laboratory Measurements of Primary Emissions and Secondary Aerosol Formation Potential of Individual Light-Duty Vehicles. Pauli Simonen, Joni Kalliokoski, Panu Karjalainen, MIIKKA DAL MASO, Topi Rönkkö, Sanna Saarikoski, Minna Aurela, Matthew Bloss, Hilkka Timonen, Georgios Triantafyllopoulos, Athanasios Dimaratos, Leonidas Ntziachristos, Zissis Samaras, Jorma Keskinen, *Tampere University of Technology*

Internal combustion engine powered vehicles produce exhaust particulate and gaseous pollutants that both affect climate and human health. Some of the emitted gaseous pollutants may produce secondary particulate mass in the atmosphere, as a consequence of atmospheric oxidation. Such secondary processes are often absent when estimating the contribution of transport to urban pollution using emission factors (EFs). Such EFs are most frequently expressed as mass of pollutant in the exhaust, normalized to the distance or fuel consumption of the vehicle concerned.

The EFs can be obtained from laboratory experiments on a chassis dynamometer or during on-road driving. While the laboratory results are highly reproducible because of the controlled environment and precisely defined vehicle operation, the emissions during engine laboratory driving cycles do not necessarily represent the emissions in real-world driving.

Here, we compare the EFs obtained from laboratory driving cycles to the ones obtained from on-road chase experiments for two EURO 6 light-duty vehicles, comprising a direct injection gasoline vehicle and a port fuel injection gasoline vehicle. In addition, on-road EFs are presented for a diesel particulate filter equipped EURO 6 light-duty vehicle. In the laboratory, NEDC and WLTC driving cycles were run on a chassis dynamometer. NO_X, CO, CO_2 and HC concentrations were measured utilizing a constant volume sampler (CVS).

During the on-road experiments, the vehicle was trailed by a mobile laboratory at a racing track where different driving patterns, including random driving were performed. For particle characterization, the mobile lab was equipped by a condensation particle counter (CPC) for particle counting. In addition, a combination of a CPC and a particle size magnifier (PSM) was used to determine the concentration of particles smaller than 3 nm in diameter. The chemical composition of the particles was measured with a soot-particle aerosol mass spectrometer (SP-AMS). Two electrical low-pressure impactors (ELPI) were used to measure the particle size distribution, and also particle mass concentration was calculated from the size distribution data. The second ELPI was measuring downstream of an oxidation flow reactor (TUT Secondary Aerosol Reactor; TSAR) to determine the secondary aerosol formation potential. In TSAR, the sample is oxidized by ozone and OH radicals, simulating atmospheric oxidation. Gas-phase emissions were measured with CO_2 and NO_X analyzers. In addition, a commercial portable emission measurement system (PEMS) was deployed during the on-road measurements to measure raw exhaust CO_2, NO_X and CO concentrations.

This study presents laboratory and on-road EFs for particle number and mass emissions, as well as the secondary aerosol production factor for the two EURO 6 gasoline light-duty vehicles, and the on-road EFs for the EURO 6 diesel vehicle. The effect of driving condition in both laboratory and on-road experiments is studied. Finally, the study discusses different methods to obtain the EF from the on-road experiment and their sensitivity to background effects.

8CB.8

Towards Monitoring Automobile Ultra-fine Particle Emissions: Size-dependent Chemical Composition. CRISTIAN FOCSA, Dumitru Duca, Jennifer Noble, Yvain Carpentier, Marin Vojkovic, Andreas Manz, Matthias Lyska, Roman Grzeszik, Torsten Tritscher, Juergen Spielvogel, Marcus Rieker, *Université de Lille*

On-road motor vehicles are important sources of ultra-fine particulate matter (PM) emissions, which present acknowledged health and environmental risks. There is currently a critical lack of certified measurement procedures for the smallest particles (< 23 nm) under real driving conditions. The development of such measurement procedures would represent an important contribution towards future particle emission regulations. The aim of the European H2020 PEMs4Nano project (www.pems4nano.eu) is to develop a portable emission monitoring system for particles below 23 nm, to be used in real driving conditions. The development of a reliable measurement procedure first requires a thorough understanding of the emitted particle characteristics (morphology, structure, chemical composition, volatility, reactivity), and their size dependence. This work presents an investigation of the chemical composition of size-selected particles emitted by a gasoline direct injection engine.

Particulate matter probed in this study was produced by a generic single-cylinder test engine (Bosch) which can be operated in various working regimes. Particles were sampled using a cascade impactor (NanoMoudi-II, MSP/TSI) which allows size-separation into 13 different size bins. Since the main interest of this work is in small particles, only the five size bins covering the range 180 to 10 nm were analysed.

Chemical characterisation of the collected particles is performed using a home-made two-step laser mass spectrometer (L2MS, Faccinetto et al., 2015). Combining gentle (low-fluence) laser desorption and various ionisation wavelengths, our instrument is able to provide detailed (nonfragmented) molecular analysis on chemical classes of critical interest, such as organosulphates, oxygenated hydrocarbons, nitrogenated hydrocarbons, and polycyclic aromatic hydrocarbons (PAHs), as well as very effective detection of heavy metals. Additional high-resolution chemical mapping is performed using a commercial Secondary Ion Mass Spectrometer (IONTOF).

The very rich mass spectra of size-selected particles require powerful statistical treatment to unveil subtle differences in chemical composition. This is done using principal component analysis (PCA) and hierarchical clustering analysis (HCA). Chemical species responsible for these variations can thus be definitively identified and the size-selected particles can be discriminated and classified according to their origin. Moreover, the influence of various experimental parameters (engine regime, fuel additives, lubricating oil, mechanical wear, etc.) can be easily identified.

The combination of mass spectrometric studies with statistical procedures reveals indisputable evidence of a size-dependence in the chemical composition of PM. This information represents critical physico-chemical data necessary for the development of a reliable portable device for the measurement of ultra-fine particles emitted by automobile engines.

This work has received funding from the European Union's Horizon2020 Programme for research, technological development and demonstration under Grant Agreement no. 724145 (H2020-GV-2016).

Faccinetto, A. et al. (2015), Environmental Science and Technology, 49, pp. 10510-10520. DOI:10.1021/acs.est.5b02703.

8CB.9

A Comparison of Partial Flow to Full Flow Dilution Tunnel Sampling for Engine Exhaust PM Measurement. MATTI MARICQ, *Ford Motor Company*

The recent CFR Part 1066 specifications ushered in as part of the US Environmental Protection Agency Tier 3 upgrades to motor vehicle emissions regulations allow the use of partial flow dilution for chassis dynamometer certification of light duty vehicle particulate matter (PM) emissions. This methodology was validated and has been allowed since 2007 for heavy duty vehicles emissions measurements, but data for light duty applications is scarce. Partial flow dilution offers a number of advantages over the traditional constant volume sampling (CVS) method, including lower cost, smaller footprint, less infrastructure, and provides an attractive pathway to upgrading vehicle emissions test cells. This methodology is not yet allowed under the new Worldwide Harmonized Light vehicles Test Procedure, being developed for use in Europe and Asia, which is one motivation for the present work.

Whereas the conventional CVS method dilutes the vehicle's entire exhaust and then samples only a very small fraction for PM measurement, partial flow dilution samples only the amount of exhaust needed for filter based gravimetric measurement (and solid particle counting if needed). This substantially reduces the size of the dilution / sampling system, but at the expense of requiring the measurement of exhaust flow and extracting a sample proportional to that flow. The present work demonstrates that a commercially available partial flow dilution system provides equivalent PM emissions results versus the traditional full flow method.

This work also examines the so-called "single filter" method. US emissions regulations are based on the composite emissions from a three part test, the Federal Test Procedure. Traditionally, this is accomplished by three PM mass measurements. But higher sensitivity and lower cost are possible by sampling the diluted exhaust from the three phases onto a single filter. We show that partial flow dilution can implement this single filter approach with higher signal to noise than the full flow dilution method. While examined here for PM, this approach works more broadly and can be applied as well to gaseous emissions, for example, formaldehyde.

8ES.1

Changes in Direct Radiative Forcing due to Differences in Marine Aerosol Size Distributions during NAAMES Field Campaigns. GEORGES SALIBA, Raghu Betha, Savannah Lewis, Chia-Li Chen, Lynn Russell, Timothy Bates, Patricia Quinn, *Scripps Institution of Oceanography*

Oceans are the largest source of biogenic particles to the atmosphere. Marine aerosols are mostly comprised of sea salt, sulfate, and organics which are efficient cloud condensation nuclei. The shape of the size distribution of marine aerosols has direct radiative effects on the climate due to light-scattering from these particles. Furthermore, changes in marine aerosols affect the climate indirectly by perturbing cloud formation, lifetime, and precipitation patterns. However, size distribution measurements from pristine marine environments are scarce. The reported data show variability and seasonal and geographical differences.

We present measurements of aerosol size distributions and chemical composition of marine aerosols measured during four consecutive North Atlantic Aerosol and Marine Ecosystem Studies (NAAMES) field campaigns. Measurements were made onboard the R/V Atlantis and cover the period from November 2015 till May 2018. These time periods were selected because they coincide with opposite extremes of the Phytoplankton life cycle, which have been shown to influence marine aerosol number and composition. We retrieved total marine aerosol size distributions by merging independent size distributions from a scanning electron mobility spectrometer (SEMS), an optical particle counter (OPC), and an aerodynamic particle sizer (APS). Our data cover the range of particle sizes from 0.01 µm to 20 µm. Single-particle chemical composition was measured using the Aerodyne high-resolution aerosol mass spectrometer (HR-AMS) light-scattering (LS) and Event Trigger (ET) modes.

The measured number and mass distributions are multi-modal with identifiable modes around 0.02 µm (Aiken mode), 0.1 µm (accumulation mode), and greater than 0.2 µm (PMA mode), in agreement with published results. Interestingly, we measured a shift to larger diameters of the size distributions measured during periods of high phytoplankton activity (2016 NAAMES) compared to size distributions measured during periods of low phytoplankton activity (2015 NAAMES). The difference was about a factor of two increase in geometric mean diameter. We are investigating the source of this shift and its implication on the aerosol direct radiative forcing. To achieve that goal, we are: (1) fitting the different modes to lognormal distributions, and (2) quantifying chemical composition from each mode using single-particle chemical information. Chemical composition constrains the effect of condensation (from oxidation of ocean-emitted gas-phase organic and inorganic precursors) on the measured size shift. (3) We are finally performing Mie theory calculations to quantify the change in aerosol scattering (and therefore direct radiative forcing) from shifting size distributions. Refractive indices, critical inputs to Mie calculations, are calculated for each particle mode using the volume-mixing rule (obtained from chemical composition information from AMS). Our results will help elucidate the aerosol direct radiative forcing in an environment that is sensitive to changes in particle number and mass.

8ES.2

The Global Distribution of Sea Salt Aerosol and Its Removal Mechanism. DANIEL MURPHY, Karl D. Froyd, Huisheng Bian, Charles Brock, Maximilian Dollner, Agnieszka Kupc, Bernadett Weinzierl, Christina Williamson, Pengfei Yu, *NOAA ESRL*

We present the first measurements of the concentration of sea salt aerosol over a wide range of latitude and altitude in the troposphere. The Particle Analysis by Laser Ionization Mass Spectrometry (PALMS) instrument measured the concentration of a wide variety of aerosol species during the deployments of the Atmospheric Tomography Mission (ATom). In particular, concentrations of sea salt were measured from near the surface to the lower stratosphere. Inferred concentrations near the surface are within the range of previous measurements. The concentration of sea salt falls off very rapidly with altitude, roughly a factor of 10 for every 2 km. This indicates efficient removal by precipitation. What sea salt was present above 4 km was notably chemically aged compared to sea salt in the boundary layer. The measured concentrations of sea salt in the upper troposphere were so small that reactions on sea salt cannot significantly affect the nitrate, sulfate, chlorine, or bromine budgets in the upper troposphere. The measured concentrations are compared to removal mechanisms in global models, with one removal parameterization overestimating sea salt aerosol in the upper troposphere by factors of up to 1000 and another matching within a factor of about 3. Making the removal of sea salt aerosol proportional to the removal of water may be an extremely simple and reasonably accurate parameterization.

8ES.3

Characterization of Haboob Dust Storms in Phoenix, AZ. PIERRE HERCKES, Denise Napolitano, Aurelie Marcotte, Jershon Eagar, Matthew Fraser, *Arizona State University*

During the summer monsoon season Arizona, very intense dust storms, or haboobs, can occur. These dust storms, characterized by a clear moving front can last from minutes to hours and can substantially impact the local air quality by a sharp increase in particulate matter (PM) and bring an influx of PM material from other locations, impacting local deposition fluxes.

During the monsoons seasons 2013 and 2014, background urban PM samples and the PM of haboob events ($PM_{2.5}$ and $PM_{>2.5}$) were collected on the Arizona State University Tempe Campus. Samples were analyzed for trace metals, organic and elemental carbon and organic molecular marker species such as polycyclic aromatic hydrocarbons (PAH) and sugars.

The PM10 concentrations in these dust storms are typically on the order of 100s $\mu g/m^3$ and can exceed 1,000 $\mu g/m^3$ for short periods of times. $PM_{2.5}$ concentrations also increase typically by a factor 5-10 compared to pre-haboob conditions. The chemical characterization shows that the dominant component of these dust storms is mineral dust, consistent with the formation mechanism of these storms as storm fronts entrain desert soil in monsoon storm outflows. However chemical analysis also shows a general increase of all species, not only crustal component. In fact elements associated with an anthropogenic activities, such as lead, cadmium, and antimony are also substantially increased in the fine particles during these events. This suggests a strong resuspension of urban and street dust. The latter is consistent with organic molecular marker species which show also a substantial increases (e.g. factor of 5 for PAH in $PM_{2.5}$). The composition data will be further discussed relative to non-haboob dust events and background urban PM.

8ES.4

The Size Distribution and Physical Characteristics of Surface Material in Iceland. MARY K. BUTWIN, Melissa A. Pfeffer, Throstur Thorsteinsson, Sibylle von Löwis, *University of Iceland*

Iceland's Highlands and South Coast are mostly made up of loose material that was created from volcanic eruptions, glacial erosion as well as the breakdown of lava fields from past eruptions over time. With large dust source areas and frequent windy conditions in Iceland it has been found that particulate matter is observed suspended in the air on average 135 days per year.

Unlike other large dust source areas such as the Sahara and the deserts of Asia, Iceland's dust sources are not as extensively studied. Past research on size distribution of potential sources for suspended material has mainly been done on volcanic ash from an ongoing eruption. Having a more comprehensive understanding of the size distribution of surface material is important when considering impacts from dust storms in Iceland. Course material can greatly decrease visibility and cause structural damage to infrastructure. Whereas, fine material can be a health risk as it is easily inhaled, this is especially true for those with preexisting respiratory conditions. The risk for respiratory distress can increase depending on the physical characteristics of the material inhaled. Fine elongated grains that can be found in volcanic ash, increase the respiratory risk as it can behave similarly to asbestos and create scar tissue in the lungs. Although this type of fibrous ash is not common in Iceland, it has been produced from multiple eruptions.

To better understand the risk dust storms, pose to Iceland's population surface samples from around the country were taken and analyzed for size, and shape. The size distribution of the surface material shows that the majority of material that can potentially be suspended has a diameter greater than 20 µm which will easily be filtered by the respiratory system and pose little risk. Due to the brittleness of the tephra some of the surface material must be breaking up into smaller particles forming PM_{10} and $PM_{2.5}$. Data from Optical Particle Counters that were at the surface supports this theory as peak concentrations occur with $PM_{2.5}$. However, when compared to the overall size distribution of potentially suspended material these fine particles make up a small percentage. Physical analysis of surface samples in Iceland are mostly consists of irregular shaped pieces of tephra, rather than elongated grains that can be found in fresh volcanic ash from some eruptions from volcanoes such as Hekla, Eyjafjajökull, and Grímsvötn. The lack of ash like particles coincides with the finding that eruptions have no long-term effect on the frequency of suspended material as much of the fresh volcanic ash either buried beneath vegetation, ice on glaciers or blown away.

8ES.6

Single Particle Measurements from Winter Fog Events in the Indo-Gangetic Plain. MICHAEL GIORDANO, Benjamin Werden, Khadak Mahata, Narayan Babu Dhital, Nita Khanal, Amit Bhujel, Sagar Adhikari, Siva Praveen Puppala, Arnico Panday, Peter DeCarlo, *Drexel University*

In the Indo-Gangetic Plain (Northern India and Southern Nepal), intense fog events have been observed during winter months. The overall composition of the fog and aerosol particles before, during, and after these events plays a crucial role in the potential heterogeneous and aqueous-phase reactions occurring over the region. These reactions can have major implications for the lifetime, transport, and human-health impacts of these intense fog events but overall composition of these particles remains unclear. This presentation focuses on single particle composition data of submicron particles obtained from a mini Aerosol Mass Spectrometer (AMS) during the NAMASTE2 campaign deployment to Lumbini, Nepal. Bulk AMS data shows a organic species dominate the mass with significant enhancements in aerosol chloride exceeding sulfate during fog events. Single particle analysis from AMS measurements, including k-means cluster analysis, is presented here to interpret mixing state of the submicron aerosol mass population.

8ES.7

Estimation of Snow Albedo Reduction due to Deposition of Light Absorbing Aerosols Using a Monte Carlo Radiative Transfer Model. DEEP SENGUPTA, Lan Gao, Eric Wilcox, Nicholas D Beres, Chiranjivi Bhattarai, Vera Samburova, Adam Watts, Andrey Khlystov, Hans Moosmuller, *Desert Research Institute*

Radiative forcing and climate change greatly depend on earth's surface albedo and its temporal and spatial variation. The surface albedo depends on the surface characteristics and ranges from 5-10% for calm ocean waters to 80% for some snow-covered areas. Clean and fresh snow surfaces have the highest albedo and are most sensitive to contamination due to deposition of light absorbing aerosols that can greatly reduce surface albedo and change overall radiative forcing estimates. Accurate estimation of snow albedo, as well as understanding of climate feedbacks from changes in snow-covered areas, is important for radiative forcing, snow energy balance, and predicting seasonal snowmelt and runoff rates. In particular, light-absorbing aerosols emitted by wildfires, if deposited onto snow surfaces, can greatly alter snow albedo and have been identified as a major contributor to regional climate forcing if seasonal snow cover is involved. However, uncertainty associated with quantification of albedo reduction by these light absorbing particles is high. Light absorbing particles can be mineral dust, black carbon (BC), brown carbon (BrC), or complex mixtures of them. So far, scientific work has focused on dust and BC and very little is known about the role of BrC.

We have applied a simple "Monte Carlo ray/photon tracing approach" to calculate the albedo of pure snow using fundamental optical constants [1]. Parametrization of single scattering parameters (i.e., single scattering albedo ω and asymmetry parameter g) of pure snow was based on fractal, droxtal, and hallow column geometries along with spheres [2]. The single scattering parameters of aerosols (emitted from Siberian peat combustion) were extracted from observation-based size distribution information and retrieved refractive index values obtained during laboratory combustion of biomass samples. Prior to any kind of multiple scattering calculation, refractive indices of both snow and impurity were internally (using the volume mixing rule of the effective medium approximation) and externally mixed (where snow and smoke aerosol particles treated separately. In our Monte Carlo Approach, we have considered multiple scattering to be the "collection" of single scattering events. Using this approach, we vary the effective snow grain size and deposited aerosol concentrations to explore the snow albedo over a wide wavelength range (200 nm – 2000 nm). Results will be compared with those of the SNICAR two-stream model (http://snow.engin.umich.edu/ snicarcode/) for snow radiative transfer to better understand the differences in snow albedo computation between plane-parallel methods and statistical Monte Carlo methods.

References

[1] Warren, S. G. and Brandt, R. E. (2008) 'Optical constants of ice from the ultraviolet to the microwave: A revised compilation', Journal of Geophysical Research Atmospheres, 113(14), pp. 1–10.
[2] Räisänen, P., Kokhanovsky, A., Guyot, G., Jourdan, O. and Nousiainen, T. (2015) 'Parameterization of single-scattering properties of snow', Cryosphere, 9(3), pp. 1277–1301.

8ES.8

Elemental Carbon Observations over Canada (2006-2015): Constraining on Regional Emissions in North America. LIN HUANG, Tak Chan, Knut von Salzen, Richard Leaitch, Sangeeta Sharma, Wendy Zhang, Darrell Ernst, Junhua Zhang, Michael Moran, Jeff Brook, Anne Marie Macdonald, Michael Wheeler, *Environment & Climate Change Canada, ASTD, Toronto, Canada*

Due to its unique physical properties, black carbon (BC) plays an important role in Earth climate system from regional to global scales. To contribute to the evaluation of models, which may help constrain regional and global emissions, an observation network of aerosol elemental carbon (EC) as BC mass has been strategically established over Canada since 2006, with most of the sites co-locating with aerosol optical observations, and GHG measurements. These sites represent different geographic locations with various continental source influences, from urban location (as Downsview /Toronto) to rural area (as Egbert, ON), then to boreal forest (as Fraserdale, ON, in eastern Canada, and East Trout Lake, SK, in western Canada) and from a high elevated site (as Whistler Mt. BC) to a remote area (as Alert, NU, an Arctic site). Because of its short atmospheric life-time, the changes in atmospheric EC concentration (specifically in seasonal and inter-annual variability) are largely reflecting the changes of emission source influences at regional scales though the impacts from atmospheric long-range transport could not be underestimated.

Weekly integrated quartz filter samples collected at these sites have been analysed for EC concentrations over the period of 2006 to 2015. Seasonal patterns and inter-annual variability of BC mass have been obtained across the sites. In comparison with several recently published emission inventories, including the historic IPCC emissions of BC for CMIP6 and Canada /US PM2.5 emissions, it is suggested that the trends observed at the sites in eastern Canada (e.g., Downsview/Toronto, and Egbert, ON) have been dominantly caused by anthropogenic emission changes and the influence from US emissions on these sites may be stronger than from Canadian emissions, whereas that the seasonal pattern and inter-annual variability observed at the sites in western Canada (e.g., ETL) have been influenced much more by biomass burning emissions. The decreasing trends (2006-2015) in eastern Canada would imply beneficial effects from clean air policies both from US (Clean Air Act) and Canada (Clean Air Regulatory Agenda) except that there are inconsistencies between seasonal patterns observed in eastern Canada and North American emissions inventories. The inconsistency reveals open questions and may suggest a possible pathway on constraining the seasonal profile of BC emissions in North America via observations.

Literatures:

[1] van Marle et al., Historic global biomass burning emissions for CMIP6 (BB4CMIP) based on merging satellite observations with proxies and fire models (1750–2015), Geosci. Model Dev., 10, 3329–3357, 2017, https://doi.org/10.5194/gmd-10-3329-2017.
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8ES.9

Aerosol Light Absorption at Different Altitudes in the European Arctic, Svalbard: The Effect of Boundary Layer Height.

Vasileios Stathopoulos, Mauro Mazzola, Christos Matsoukas, KONSTANTINOS ELEFTHERIADIS, *NCSR Demokritos, Athens, Greece*

Hourly measurements of aerosol light absorption coefficient, measured with an AE-31 aethalometer (550 nm) at the highly elevated Zeppelin (474 m asl) and with a Particle Soot Absorption Photometer (PSAP, 530 nm) at Gruvebadet (40 m asl) stations, are studied for one and a half year period. The height of the Planetary Boundary Layer (PBL) is estimated, for the same period, with the Liu and Liang method (Liu et al, 2010), from daily radiosonde data. The radiosonde data are obtained from the Ny-Ålesund homogenized radiosonde record, available from Maturilli et al, 2016. The correlation of the time-series is examined for different seasons, with respect to the relative position of the stations inside or outside the first Surface Layer within the PBL. This methodology investigates the possibility of assessing simultaneous light absorption measurements associated with light absorbing carbon from the lower and the free troposphere. We observe that the frequency of a surface layer engulfing both measurement stations is more common in the summer than winter. In general the gradient of the absorption coefficient with height remains significant both in the case of a single layer or two decoupled layers within the first 500 meters. However, the case of distinct layers with different aerosol light absorption appearing in the free troposphere decoupled from the surface layer appears more frequently in the winter than the summer, an observation consistent with the general circulation patterns expected in the Arctic.

8IB.1: KEYNOTE

Melioidosis from Aerosolization of the Environmental Bacterium Burkholderia Pseudomallei. BART CURRIE, *Menzies School of Health Research & Royal Darwin Hosp., AU*

Melioidosis is caused by infection in humans and animals with the soil and water bacterium Burkholderia pseudomallei. While traditionally endemic in Southeast Asia and northern Australia, improvements in surveillance and diagnostics have increasingly unmasked cases of melioidosis and the presence of B. pseudomallei in local environments in the tropics and subtropics globally, including in the Americas and most recently Puerto Rico.

The Darwin Prospective Melioidosis Study has enrolled all culture-confirmed cases of melioidosis from the tropical Top End of the Northern Territory of Australia since October 1st 1989. With 1052 cases over 28 years, annual incidence rates are strongly influenced by rainfall and wind, being over 50/100,000 in some recent years with concomitant rates in the Indigenous population of over 100/100,000. Around 85% of cases present with acute illness, with the likely infecting event being increasingly identified through informed patient history and occurring within the 3 weeks prior to symptom onset. Recognised examples of exposure events that have been documented include inhalation or percutaneous inoculation during high pressure hosing or while mowing lawns or using a whipper-snipper (weed-whacker). Pneumonia is the presentation for half of cases, overall bacteremia rates are 60% and septic shock occurs in 21% of all cases, with most requiring ventilation in the ICU. With current treatment guidelines relapsed melioidosis is now very uncommon and mortality in Darwin has fallen from initially over 30% of all cases to around 10% in recent years. Nevertheless mortality from melioidosis remains over 40% in many regions globally where there are no or limited diagnostic laboratory capabilities, lack of the antibiotics required for optimum therapy (ceftazidime and meropenem) and no state-of-the-art hospital facilities for managing patients with severe sepsis.

What remains totally unclear is the proportion of cases that are from aerosol inhalation of B. pseudomallei in comparison to percutaneous inoculation or ingestion, with clinical (e.g. mediastinal disease) and epidemiological data from the Darwin study supporting but not proving a shift to inhalation during severe monsoonal weather. While activation from a latent focus is a rare occurrence, the proportion of those asymptomatic but seropositive to B. pseudomallei who have latent bacteria still present with the potential for later activation (the “Vietnamese Time Bomb”) also remains entirely unclear.

Air sampling studies have only occasionally successfully cultured B. pseudomallei from samples taken during weather events. In one Darwin case of severe melioidosis with pneumonia and mediastinal mass, whole genome sequencing of a positive air sample B. pseudomallei isolate collected outside the patient’s accommodation was closely matched to the sequence of the clinical isolate from the patient’s blood culture.

Various rodent and primate animal models have been used to study the aerosol route of infection with B. pseudomallei. They provide support to the proposition that deliberate release of manufactured B. pseudomallei aerosols in a high density city population could have catastrophic consequences analogous to those from anthrax and justifying the listing of B. pseudomallei as a Tier 1 Select Agent.

8IB.3

Aerodynamic Particle Size Affects Infectivity and Lethality, but not Disease Timecourse, in a Nonhuman Primate Model of Inhalational Melioidosis. JEREMY BOYDSTON, John Yeager, Artemas Herzog, Jill Taylor, David Dawson, Angelo Scorpio, Paul Dabisch, *BNBI / DHS NBACC*

Burkholderia pseudomallei, the causative organism of melioidosis, is endemic in Australia and Southeast Asia. While percutaneous inoculation is believed to be a major route of exposure, but recent studies have detected B. pseudomallei in air samples collected during typhoon season suggesting that inhalation may also be a natural route of exposure. While the particle size distribution of naturally occurring aerosols containing B. pseudomallei has not been measured, measurements of naturally occurring aerosols containing other microorganisms suggest a wide range of particle sizes are possible. For many pathogenic microorganisms, there is evidence that aerodynamic particle size is a significant factor influencing the disease presentation and lethality. Therefore, the aim of this study was to determine the influence of aerodynamic particle size on the disease presentation and median lethal dose in a nonhuman primate model of inhalational melioidosis. The results demonstrate that infectious and lethal doses were significantly greater in animals exposed to large particles (MMAD: 11.5 µm, GSD: 1.27) versus small particles (MMAD: 1.5 µm, GSD: 1.39). It is likely that the observed difference between the two groups is due to differences in the regional deposition pattern of the inhaled aerosol. Interestingly, the median time to death, median time to fever, and cytokine responses did not differ between infected animals in the two particle size groups. Minor histopathological differences were also noted between the groups, including an increased incidence of inflammation in the olfactory bulb in non-survivors in the large particle exposed group and a decreased incidence of severe lung inflammation in survivors in the large particle exposed group, but the significance of either histopathological difference to outcome cannot be assessed without additional studies. Taken together, these results suggest that once infection is initiated, melioidosis disease progression is largely independent of differences in aerodynamic particle size and associated differences in pulmonary deposition patterns. Additionally, the results of this study highlight the need for future studies in which the particle size distribution of naturally occurring aerosols containing B. pseudomallei is measured.

All research was conducted in compliance with the Animal Welfare Act and other federal statutes and regulations relating to animals and experiments involving animals and adheres to principles stated in the Guide for the Care and Use of Laboratory Animals. The facility where this research was conducted is fully accredited by the Association for Assessment and Accreditation of Laboratory Animal Care International.

8IB.4

Pulmonary Delivery of Ceftazidime for the Treatment of Melioidosis in a Murine Model. SARA RUIZ, Larry Bowen, Mark Bailey, Cory Berkland, *USAMRIID*

Interest in *Burkholderia pseudomallei*, the causative agent of melioidosis, has increased over the years given its status as a select agent. This is due to its inherent ease of aerosol transmission, resistance to common antibiotics, and ability to establish both an acute and chronic infection. Clinical manifestations range from pneumonia to acute sepsis with chronic individuals being asymptomatic for a number of years before progressing to acute disease. To date, there is no vaccine available for melioidosis and even with the proper antibiotic course of treatment, therapy fails in approximately 10% of patients. In vitro studies have shown that *B. pseudomallei* is able to form biofilms readily. Other medically important bacteria, including *Staphylococcus aureus*, have shown biofilm formation as a contributing factor to overall virulence including antibiotic resistance and chronic disease. We have demonstrated that biofilms can be visualized in non-human primate lungs infected with *B. pseudomallei* upon staining with fluorescent markers. In addition, all strains secrete known quorum sensing effectors that influence biofilm formation as determined by liquid chromatography tandem mass spectrometry (LC-MS/MS). The presence of a biofilm during the natural course of disease implies that it is an important bacterial state to consider in assessing novel treatment options. Inhaled antibiotics are a promising avenue to pursue for pulmonary diseases, including biofilm infections. Ceftazidime was delivered via a nose-only system to BALB/c mice challenged with *B. pseudomallei*. Mice treated with nebulized ceftazidime became symptomatic but survived until study end, which was comparable to those treated intraperitoneally. Upon necropsy, bacteria remained within the spleens of the majority of the experimental animals. The effectiveness of nebulized ceftazidime warrants additional studies to improve the treatment regimen and to test as a prophylactic therapy against *B. pseudomallei.*

8IB.5

Defining Pathogen Transmission Risks during Aerosol Generating Procedures in Healthcare Settings. Jiayu Li, Carrie O'neil, Ramesh Raliya, Yang Wang, Anna Leavey, Meghan Wallace, Carey-Ann Burnham, Adrianus Boon, HILARY BABCOCK, Pratim Biswas, *Washington University in St Louis*

Questions remain about the degree to which aerosols are generated during patient-care activities and whether generated aerosols could transmit viable pathogens to healthcare personnel or to other patients. We measured aerosol production during common patient-care activities and collected samples for pathogen recovery. Some patient-care activities were included: patient bathing, changing bed linens, pouring and flushing liquid waste, bronchoscopy (with and without negative pressure ventilation), non-invasive ventilation, nebulized medication administration, extubation, and mechanical ventilation. Multiple aerosol characterization instruments were used to measure aerosols generated during each procedure. SKC BioSamplers were used for pathogen recovery[1], along with a NIOSH personal aerosol sampler and a viable virus aerosol sampler (VIVAS) for a small subset of samples. All samples were subjected to bacterial culture. Samples collected from patients known to have influenza also received viral culture. During the first stage of the study, patients on contact precautions for drug-resistant organisms were prioritized for sampling[2]. In the second stage of the study, patients with influenza or other respiratory viruses were prioritized for sampling. Baseline samples were collected when possible. Results of both stages of the study indicate that nebulized medication administration and bronchoscopy with nebulized medication administration generated a significant change in particle presence over baseline. For the first stage of the study, of 78 samples subjected to bacterial culture, 18 were positive for clinically insignificant bacteria, however, none of the targeted drug-resistant organisms were recovered. The most frequently isolated organism was coagulase-negative *staphylococcus*, followed by *micrococcus,* which are common environmental contaminants, rather than targeted pathogens. For the second stage of our study, although none of the samples have been positive for the respiratory virus, similar to the first stage of the study, we have had several bacterial cultures that were positive for normal skin/environmental bacteria.

Strengths of this study include the use of multiple real-time aerosol measurement instruments, use of culture to determine the presence of viable microbes as a metric to assess the infection risk posed by medically generated aerosols, testing for viral pathogens during the second round of sampling, and sampling during multiple types of medical procedures in a real-world healthcare setting. Although additional research is needed, the results of this study suggest that some of the procedures that are widely considered to be high risk for the generation of infectious aerosols may actually pose little infection risk to protect healthcare personnel (HCP).

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8IB.6

Overview of Tuberculosis Transmission by Aerosol. CHAD J. ROY, *Tulane University*

There are few other pathogens that has made a deeper, lasting impression on our species than Mycobacterium tuberculosis (Mtb), with evidence of the first human infections taking place over 20,000 years ago. Tuberculosis is important in the human interface as the disease classified as one of the worlds' only requisite obligate respiratory pathogens; that is transmission of most all tuberculosis disease is initiated though proximity contact with an infected host and the airborne transfer of infectious bacilli to a susceptible host. Despite the longevity of tuberculosis as a disease of the human condition, we collectively only recognize few clear indicators of the requirements associated with natural aerosol infection with Mtb and whether the evolution of the bacilli as recalcitrant to the environment is primary or corollary to resulting infection rates among susceptible populations. Scant data is available on aerosol-centric details of transmission of tuberculosis, including the magnitude of infectious particles generated and number of which is contained in normal exhalation, cough/sneeze or other violent expulsion from the host, and if particle size distribution that is exhaled is within a size consistent with respirability or inhalability and presence of viable bacilli. Similarly, little is known of the potential of bacilli-laden particles within these distributions to overcome physiochemical stressors such as dehydration and ultraviolet natural degradation during environmental transport between the infected and naïve host. Once inhaled, the dose requirement for induction of disease in a susceptible host is simply unknown – yet it is widely accepted that Mtb infection is not considered a purely stochastic event and rather requires some multiplicity for successful infection to take place. It is clear that a deep understanding of the aerosol transmission of tuberculosis and characterization of the major variables that influence infection remain an open question despite the contributions of historically relevant research that explored the 'droplet nuclei theory of airborne contagion'. A number of notable current studies as well share the goal of bringing evidentiary detail to the phenomena of airborne transmission of tuberculosis. The collective of past and current research upon the modern theory of Mtb transmission all within the context of bioaerosol dynamics will be discussed in this presentation.

8IB.7

Capture and Characterization of Exhaled Bio-aerosols from Tuberculosis (TB) Patients. ROBIN WOOD, Carl Morrow, Benjamin Patterson, Wayne Bryden, Charles Call, David Silcott, Catherine Fenselau, D. Chen, R. Dinkele, S. Gessner, Digby Warner, *IDM, University of Cape Town*

The respiratory aerosol sampling chamber (RASC) was designed to create a safe, contained environment for bio-aerosol investigation of the production of Mycobacterium tuberculosis (MTB) bacilli by individual tuberculosis (TB) patients. Key design features include the small volume (1.4m^3), HEPA filtration of inflowing air with continuous monitoring of temperature, relative humidity, carbon dioxide concentrations, airborne particle concentration, and cough frequency. Scanning electron microscopy studies of impacted particles revealed occasional MTB-like organisms, and solid medium culture produced colonies of confirmed MTB with detection efficiency of 43%. Here, we detail efforts to make further improvements on the sensitivity of the collection and detection systems.

Sampling system: The optimized collection of bio-aerosol uses a single, large air volume (250L/m) sampling cyclone (Bertin Coriolis μ™) and liquid collection. The liquid sample containing collected bio-aerosol is centrifuged followed by mass spectrometry of the supernatant and bacteriological assay of the pellet via fluorescence microscopy.

Mass spectrometry: The mass spectrometry (Thermo Fisher, Orbitrap LTQ™) protocol developed in the pilot study resulted in a putative TB diagnosis from bio-aerosol sampling with a rapid (1-2 day) turnaround. Moreover, the diversity of lipids discovered to date indicates that correlates may be developed that provide more detailed information about the disease state. There is also the potential for discovery of specific diagnostic markers in human breath that could be measured more rapidly using less complex protocols. It is proposed that simplification of the process may lead to a readily fieldable diagnostic.

The liquid-capture pellet is re-suspended and distributed over a microscope slide containing multiple single nanoliter-sized wells. The spatially separated MTB within the nano-wells are then stained with a recently described fluorescent trehalose dye which is incorporated into the cell walls of viable, metabolically active bacteria. Quantitative detection of these organisms is enabled by fluorescence microscopy, with current efforts aimed at developing time-lapse imaging for additional phenotyping including growth rates.

Bio-aerosol from TB patients can be collected in the RASC. Viable MTB organisms can be rapidly imaged using a non-destructive assay and specific mycobacterial lipids detected by mass spectrometry.

8IB.8

Exploring the Fundamentals of Biological Decay and Survival in Aerosol Droplets with a New In Vitro Technology.

MARA OTERO-FERNANDEZ, Allen E. Haddrell, Jonathan P. Reid, Richard Thomas, *University of Bristol*

Understanding the parameters that determine the longevity of microorganisms during atmospheric transport is critical for public health and biodefense applications, ranging from outbreak control to risk analysis modelling. The study of bioaerosols in a laboratory environment is challenging and requires careful consideration of each experimental phase:

(1) Quantifying the complete droplet composition, from the individual to the population level, while minimizing microbial damage during the aerosolization process (Zhen et al. 2014).
(2) Complete control over the atmosphere (e.g. temperature, relative humidity) where the droplets are suspended whilst avoiding physical loss of the particles.
(3) Minimizing stresses that occur during aerosol sampling.

Conventional techniques for investigating the survival of bioaerosols in vitro have some limitations that can impact the accurate representation of conditions that these particles would experience in the environment. Therefore, some basic questions about the fundamentals of airborne disease dynamics remain unknown.

In this study, a recently developed technology that utilizes a droplet-on-demand aerosol generator to produce a tailorable number of bioaerosol droplets with designed composition, without compromising the microorganisms' viability, will be demonstrated. These droplets are suspended in an electrodynamic trap where the internal atmosphere is highly-controlled regarding atmospheric parameters and chemical composition. After the desired suspension period and throughout manipulation of the electric field, the droplets are deposited onto a subtract with a high efficiency and time-resolution. By manipulating the substrate, the dissociation between viability and infectivity of the airborne pathogens contained within the droplets can be studied.

The findings to be presented will demonstrate some of the unique characteristics of this technique including:

a) The characterization of the first phase of cell death, achievable due to the high time-sampling resolution (under 10 seconds).
b) Longevity measurements of populations of droplets (whose absolute number can be readily counted) with accurate microbial and chemical composition. Correlations between the complete aerosol composition/concentration and longevity (with no physical loss component) will be explored.

Zhen, H. J. et al, G. J Aerosol Sci. 2014;70,67-79.

8IB.9

Studying Survival of Aerosolised Bacteria Using Poly(methyl) Methacrylate Microthreads. ANDREW SCOTT, Carwyn Davies, Emma Keyser, *Dstl*

Appreciating the hazard posed by airborne infectious agents is crucial to allow planning and implementation of effective impact-mitigation strategies for military and civilian first responders. In order to understand the potential downwind hazard following a release of a biological agent it is necessary to define the aerosol survival characteristics of each agent under a range of environmental conditions. Experimental determination of aerosol survival in the laboratory can be challenging, particularly with the added physical constraints and biosafety and engineering requirements of studying high-containment pathogens. To address some of these challenges, one approach is to use poly(methyl) methacrylate microthreads to capture pathogen-containing particles from an aerosol. Once captured, the particles are stably held by the microthreads and appear to behave as if they were still suspended in the air. The benefit of this system is that it allows the captured particles to be easily moved and placed in environmental conditions which might otherwise be inaccessible using the traditional methods of maintaining buoyant aerosols, such as the rotating drum. However, the establishment of this technique has not been without its own complications. Here we will present our work to establish and validate the fundamental limits and parameters of the microthread technique, its potential for establishing survival characteristics in varying environmental conditions in the laboratory and how some critical validation studies might be undertaken, in particular examination of the survival characteristics of non-pathogenic reference microorganisms to allow benchmarking of the results gained in the laboratory.

8IM.1

Overview of the First In-situ Intercomparison of Aerosol Photoacoustic Spectrometers. CHRISTOPHER ZANGMEISTER, James Radney, *National Institute of Standards and Technology*

We describe results from the first intercomparison of aerosol photoacoustic spectrometers using a carbon black material. Data was collected by 12 laboratories located across North America, Europe and Asia. Absorption cross sections were measured using a well-defined, easily dispersible material distributed by the National Institute of Standards and Technology (NIST) to each participating laboratory, enabling the assessment of the variability in aerosol absorption measurements under well-controlled laboratory settings at each participants home institution. The participating laboratories measured aerosol absorption cross sections, of mobility and, if possible, mobility and mass selected aerosols. The data was reported in terms of absorption cross-section per particle or the mass-specific absorption cross section (MAC). The data will be discussed in terms of the comparability of data across all participating laboratories and as a function of the methods of particle selection (i.e. mobility versus mobility and mass) and wavelength. We envision, the results generated from these data will enable best practices to be developed by the community for the calibration and operation of aerosol photoacoustic spectrometers.

8IM.2

MultiPAS-IV: A Portable, Four-wavelength Photoacoustic Spectrometer for Ambient Aerosol Absorption. GEOFFREY SMITH, Al Fischer, *University of Georgia*

We have developed a portable, four-wavelength, single-cell photoacoustic spectrometer for simultaneous measurement of aerosol absorption at 406, 532, 662, and 785 nm, with an additional extinction measurement at 662 nm via a built-in cavity ringdown spectrometer. The instrument, dubbed MultiPAS-IV, is compact, robust, has low power requirements, and utilizes a multipass optical arrangement to achieve typical detection limits of 0.6 – 0.7 Mm^{-1} for absorption (2σ, 2-minute average).

Tests with size-selected nigrosin aerosols show agreement with Mie theory calculations to within 2%. Comparison with a 7-wavelength aethalometer shows good correlation but poor agreement for ambient (Athens, Georgia) aerosols, indicating potential multiple scattering artifacts with the filter-based aethalometer.

We demonstrate the utility of the broad spectral coverage and sensitivity of the MultiPAS-IV for calculating the absorption Ångström exponent of black carbon ($AÅE_{BC}$, median value of 0.70) in ambient aerosols. Importantly, the single cell design of the instrument allows this value to be derived independent of calibration. The $AÅE_{BC}$ is also used to derive the contribution of brown carbon to absorption at 406 nm (43%) and 532 nm (13%) and its wavelength dependence ($AÅE_{BrC}$ = 6.3).

8IM.3

Counting Efficiency Evaluation of Optical Particle Counters in Micrometer Range by Using Inkjet Aerosol Generator.

KENJIRO IIDA, Hiromu Sakurai, *AIST*

It is challenging to aerosolize PSL spheres whose diameter is greater than 1 µm and use them to evaluate the counting efficiencies of optical particle counters (OPCs). Particle number concentration of PSL spheres tend to drift during nebulization of liquid suspension or strongly fluctuate during dry-dispersion. Instead of aerosolizing PSL spheres previous studies often use a monodisperse aerosol generator such as vibrating orifice aerosol generator to generate test particles whose diameter is greater than 1 µm.

Regardless of the particle material the parallel comparison method has been used to evaluate the counting efficiencies of OPCs, η. During the evaluation of η the OPC under test (hereafter the DUT-OPC) samples from a distributing box a well-mixed aerosol of test particles in parallel with a reference instrument. The η is determined as the ratio of the number concentration reported by the DUT-OPC to that reported by the reference. The parallel comparison method requires that test particles are well-mixed in a distribution box and transported to the DUT-OPC and a reference instrument. However, the particles above 1 µm may not mix well in the distribution box, and also their losses in the transfer tubes from the distribution box may be different between the tube to the DUT-OPC and that to the reference. This effect becomes more significant as the difference in the sampling flowrate between the DUT-OPC and the reference increases.

This study introduces the method to evaluate the η at particle diameter greater than 1 µm by using Inkjet aerosol generator (IAG). The IAG-based method defines the η as ratio of the particle count rate of a DUT-OPC to the particle generation rate of the IAG. This count-rate-based η can be converted to a concentration-based value if the true flowrate of the DUT-OPC is known or measured. This study demonstrates the evaluations at 5 µm and 10 µm in volume equivalent diameter. The chemical composition of the particles are either sodium chloride (SC) or lactose monohydrate (LM). The aerosol flowrate of the IAG is set at 0.3 L/min, and the aerosol is delivered to an OPC (ZN-PD50-S, OMRON, Japan) whose sampling flowrate is 6 L/min and minimum detectable size can be set at either 5 µm or 10 µm. The mismatch of the flowrates is compensated by adding particle free-air in a laminar flow chamber.

In order to simulate the sampling of uniformly mixed aerosol from a real environment the particles are delivered to different points over the inlet plane of the isokinetic probe attached to the OPC. Particle flux into the isokinetic probe is proportional to the gas-velocity into the probe; however, the true velocity distribution is usually unknown. It is assumed that the true velocity distribution is bounded by two flow models: the plug and parabolic flows. A set of delivery points are prepared to simulate the particle flux under each flow model.

Experimental results show that the choice of flow model influences the value of η at 10 µm indicating the η is potentially different from the true value since the true value can be evaluated only if the true velocity distribution is known. The potential bias in is considered as a source of systematic error in our uncertainty analysis. When the minimum detectable size of the OPC is equal to the volume equivalent diameter of the test particles the value of η strongly depends on the particle material, and the greater fraction SC particles are detected since their PSL-equivalent optical diameter is greater than LM particles.

8IM.4

A Single-pass RGB Differential Photoacoustic Spectrometer for Aerosol Absorption Measurement. ZHENHONG YU, Gregory Magoon, William Brown, James Assif, Richard Miake-Lye, *Aerodyne Research, Inc.*

We developed a single-pass RGB photoacoustic spectrometer for aerosol absorption measurement at 671nm (red), 532nm (green) and 473nm (blue). This instrument uses the differential photoacoustic absorption spectroscopic (DPAS) technique, in which signals due to light absorption of total PM + gaseous samples and those of gaseous samples alone are measured simultaneously in two identical acoustic cells. The difference between the photoacoustic signals yields the aerosol absorption coefficients at the three wavelengths. This measurement approach eliminates the interferences from the light-absorbing gaseous species as well as the surrounding low-frequency background acoustic noises.

In this design, laser beams of three diode-pumped solid state lasers at the RGB wavelengths with superb beam quality were merged into a single beam via dichroic mirrors before passing through the photoacoustic cells. The laser beam at each color was amplitude modulated separately at 50% duty cycle around the resonance frequency of the photoacoustic cells via a square-waveform control on their electrical DC power controls. Frequency-division multiplexing was used to combine the three-color photoacoustic signal, allowing simultaneous absorption monitoring at the three wavelengths. To accomplish that, the modulation frequencies were slightly different by approximately 5 – 15 Hz.

Custom-designed miniature microphone array detectors were used to measure photoacoustic signals at each cell. Each detector contained four silicon-based microelectromechanical system (MEMS) microphones, which were integrated onto a printed circuit board with voltage regulators, band-pass filters and low-noise voltage preamplifiers.

Data acquisition for the RGB DPAS system was carried out via a fast-response and high-resolution DAQ device, in which an analog-to-digital converter (ADC) was used to convert the analog voltage outputs from the PCB into 24 bit-resolution digital outputs for digital signal processing. Instead of using the conventional phase-sensitive detection scheme, we utilized least-squares (LS) analysis to extract signal parameters.

Signal responses of the RGB DPAS instrument were calibrated with mono-disperse carbon black samples. Based on the Allan variance analysis, detection sensitivities (2δ) of 0.3 Mm^{-1} at 671nm, 0.3 Mm^{-1} at 532nm and 1.2 Mm^{-1} at 473nm have been achieved in 100s data acquisition for the RGB DPAS instrument. The single-pass configuration allows us to determine aerosol absorption angstrom exponent (AAE) directly from photoacoustic signals and laser power measurement, without calibration of signal response.

8IM.5

Experimental Determination of Aerosol Growth Kinetics via Simultaneous Measurement of Constant Angle Mie Scattering Pattern at Two Different Wavelengths. MIGUEL VAZQUEZ-PUFLEAU, Paul M. Winkler, *Universitaet Wien, Vienna, Austria*

Understanding aerosol formation and growth is essential for better quantification of climate and health effects, the design of catalysts, nano-electronics and novel nanomaterials with tuned morphology. However, the study of the kinetics and mechanism for the initial stages of aerosol growth in the free molecule regime has been limited in the past due to the difficulty to measure aerosol growth in this size regime with sub-millisecond temporal resolution. To tackle these difficulties, the so-called constant-angle Mie scattering (CAMS) instrument was developed (Wagner, J. Colloid Interface Sci., 1985, 105(2): 456-467). This instrument provides growth rate of monodisperse particles, as well as total number concentration based on a laser and optical detectors. The measurement is done, in an expansion chamber where supersaturation is induced by adiabatic expansion of an initial vapor mixture at well-defined conditions. Such features make the CAMS method ideal for in situ measuring growth rates of aerosols from supersaturated vapor. The CAMS principle has been demonstrated in the past using single lasers with visible light (Pinterich, Aerosol Sci. Technol., 2016, 50(9): 947-958.; Winkler, Phys. Rev. Lett., 2004, 93(7): 075701), allowing growth rate measurements in the continuum regime, around a few microns.

The smallest particle size that can be detected using the CAMS method is given by the first Mie maximum in the scattering plot. Subsequent patterns in the signal are used to compute larger size parameters based on Mie scattering theory. Particle growth rate can then be directly computed by matching theoretical peaks to the experimental scattering plot that is measured as a function of time. Since the size parameter given in Mie theory is defined as the ratio of droplet size over wavelength, a direct way to lower the detection limits of the instrument is to use a laser with a smaller wavelength. However, when using adiabatic expansion, smaller particles tend to grow faster than larger particles and determining the first peak as well as obtaining well separated subsequent peaks becomes increasingly difficult.

In this work, we aim to provide aerosol growth rate measurements in the free molecular regime by incorporating an additional laser, perpendicular to the first one and with a smaller wavelength. The narrower wavelength allows the measurement of smaller particles and having two independent particle size measurements allow temporal cross-comparison. This triangulation provides more accuracy and reliability on the whole range of the measurements, even beyond the overlapping region. This research has the potential to open exciting new applications and provide useful evidence for better understanding the initial stages of aerosol growth.

8IM.6

Morphology and Comparisons of BC Mass Concentrations Measured by LII, CAPS, and PAX of PM Emitted from a Grand Cherokee and a Ford F-150 under Different Drive Cycles. FENGSHAN LIU, Fadi Araji, Greg Rideout, Prem Lobo, Gregory Smallwood, *National Research Council Canada*

Combustion-generated ultrafine particulates pose a serious concern for human health and climate warming. These nano-sized particles, when inhaled, are able to penetrate deep into the lungs and onto organs. Their black carbon (BC) component is strongly light-absorbing and has a strong climate warming effect. To establish a reliable BC inventories and evaluate BC mitigation techniques such as after-treatments and novel design of combustion devices or fuel technology, it is paramount to develop capabilities for real-time and accurate BC mass concentration measurements. BC aerosols contain different levels of elemental carbon (EC) and organic carbon (OC), depending on the combustion conditions and fuels. Various BC mass measurement instruments, which were developed based on a specific phenomenon of light and matter interactions, have been developed and extensively deployed for BC mass measurements. Unfortunately, there exists fairly large uncertainty in BC mass concentrations measured by various instruments, since they respond differently to variations in the physical (size, morphology, and the micro-structure) and chemical (EC/OC ratio) properties of the BC containing particles.

In this study, the BC mass concentrations of particulate matter (PM) emitted from two light duty trucks operated on a chassis dynamometer under different drive cycles were measured using a cavity-attenuated phase shift (CAPS) PM_{SSA} monitor (at 660 nm), a photoacoustic extinctiometer (PAX) (at 870 nm), and an Artium LII 300 based on the laser-induced incandescence (LII) technique. The vehicles tested were a port fuel injection (PFI) Jeep Grand Cherokee and a gasoline direct injection (GDI) Ford F-150. During each test, the vehicle exhaust was directed into a Code of Federal Regulations compliant (CFR 1065) full-flow constant volume sampling system and diluted with high-efficiency particulate air (HEPA) filtered room air. The diluted exhaust was measured by CAPS and PAX, while the BC mass concentration measurement by LII300 was made in the undiluted exhaust directly from the vehicle tailpipe. The dilution ratio was evaluated by monitoring the CO2 concentrations. To help understand the potential differences in the mass concentrations measured by the different instruments, an ESPnano sampling device was also deployed to collect PM particles on 3-mm copper grids for TEM imaging and subsequent analysis for particle morphology.

The objective of this study is to understand the relative performance of the three tested real-time BC mass instruments applied to vehicle emissions under different drive cycles. The differences in the measured BC mass concentrations measured by CAPS, PAX, and LII are discussed in terms of the particle morphology, the level of concentration, and the drive cycle, which affects the combustion mode and hence the EC/OC ratio and carbon atom structure. In addition, the absorption coefficients measured by CAPS and PAX are used to infer the Ångström absorption exponent (AAE) of PM aerosols emitted from the two trucks at different drive cycles.

8IM.7

Determination of the Effect of Lens Fouling of the CAS-POL for the Measurement of Airborne Float Coal Dust. CLARA E. SEAMAN, Michael R. Shahan, *National Institute for Occupational Safety and Health*

Float coal dust (FCD) is defined as coal dust particles smaller than 75µm that are generated by various mining operations and transported by ventilating air until settling in the mine entries. FCD has been identified as an explosion hazard in coal mines, contributing to 18% of U.S. coal mining related fatalities between 2001 and 2010. The main mitigation of this hazard is the application of rock dust. Water sprays may be used as an additional method for controlling FCD by preventing it from leaving the mining face. Traditionally, gravimetric techniques are used for evaluating the effectiveness of water spray controls. However, gravimetric measurements are only able to provide a shift average efficiency measurement and are unable to provide insight into the size distribution of FCD. The Cloud Aerosol Spectrometer with Polarization (CAS-POL) has been successfully used in NIOSH pilot studies to determine the efficiency of a single spray in open space. During this testing, a reduction in the dust concentration as measured by the CAS-POL was observed over the course of a day even though the dust source was held constant. It is believed that this shift in the dust concentrations measurements may be linked to the buildup of dust on the CAS-POL lenses. This study was designed to determine the impact of lens fouling on the CAS-POL data and to establish guidelines for cleaning the lenses in order to minimize measurement errors due to fouling.

For this investigation, the CAS-POL was centered in the Pittsburgh Mining Research Division longwall gallery and subjected to different types of dust loading. During each loading test, the dust was cycled on for 30 minutes and off for 3 minutes to establish baseline values for the CAS-POL as the lenses were loaded with dust. Tests were varied by length and type of dust used. It was observed that during a test the total number of particles detected in a cycle did not change significantly over time, but total weight significantly decreased. When particles were segregated by size fractions, the number of small particles ($D \leq 4$ µm) increased while the number of larger particles (4 µm $< D \leq 20$ µm and $D>20$ µm) decreased significantly. Using the sizing data to estimate mass, all three size fractions decreased significantly over time following a linear decease for small particles and a power relationship for larger particles. The change in particle count and mass for both size fractions is correlated to the sizer high baseline value, one of the CAS-POL housekeeping variables, which increases linearly in response to length of dust exposure. Together these results suggest that lens fouling leads to an increase in sizing errors which can be monitored using the sizer high baseline value. Further analysis will focus on determining an acceptable threshold for the sizer high baseline value which will be used to indicate the need to clean the CAS-POL lenses.

8IM.8

Data Inversion Methods to Determine Sub-3 nm Particle Size Distributions Using the Particle Size Magnifier. RUNLONG CAI, Dongsen Yang, Lauri R. Ahonen, Linlin Shi, Frans Korhonen, Yan Ma, Tuukka Petäjä, Jun Zheng, Juha Kangasluoma, Jingkun Jiang, *Tsinghua University*

Measuring particle size distribution accurately down to approximately 1 nm is needed for studying atmospheric new particle formation. The scanning particle size magnifier (PSM) using diethylene glycol as the working fluid has been used for measuring sub-3 nm atmospheric aerosols. A proper inversion method is required to recover the particle size distribution from PSM raw data. However, the performance of PSM inversion methods, especially considering the influence of random errors, has not been systematically examined. Similar to many other aerosol spectrometers and classifiers, PSM inversion can be deduced to a problem described by the Fredholm integral equation of the first kind. The inversion methods used in other aerosol instruments can possibly be applied to solve the PSM inversion problem. Among them, those methods requiring with less prior information on the particle size distribution are more preferable.

We tested the performance of the step-wising method, the kernel function method (Lehtipalo et al., 2014), the H&A method (Hagen and Alofs method, 1983), and the expectation-maximization algorithm. The step-wising method and the kernel function method were used in previous studies on PSM. The H&A method and the expectation-maximization algorithm were used in data inversion for the electrical mobility spectrometers and the diffusion batteries (Maher and Laird., 1985), respectively. In addition, Monte Carlo simulation was used to test the accuracy and precision of the particle size distributions recovered using different inversion methods. The relative random errors estimated from atmospheric observation and laboratory study were added in the simulated particle concentration detected by the PSM. Laboratory experiments were conducted to test the sizing accuracies of different inversion methods and to verify the results predicted by the simulation.

The step-wising method may report false sub-3 nm particle concentrations when there are no sub-3 nm particles because it does not account for the influence of particles large than 3 nm. The kernel function method and the H&A method may lead to relatively large uncertainties in the recovered particle size distribution because of using the unstable least square method. Sometimes they report false sub-3 nm concentrations due to the large uncertainties. Compared to the kernel function method, the H&A method lead to smaller uncertainties while having similar computational expenses. Among all the tested inversion methods, the expectation-maximization algorithm has the highest accuracy and stability. We suggest using the expectation-maximization algorithm to retrieve the particle size distributions from PSM raw data. The H&A method is recommended for preliminary analysis considering the computational expenses of the expectation-maximization algorithm.

Based on the inversion analysis, we also provided practical suggestions on PSM operations. The uncertainties of the recovered size distributions of particles smaller than 1.3 nm or larger than 3 nm may be large due to the incomplete kernel function curves, the low resolutions, and/or the low detection efficiencies. The measuring uncertainties in the scanning mode may also increase the uncertainties of the recovered size distribution. Thus, the scanning scheme of the saturator flow rate is suggested to be improved to reduce the measuring uncertainties. In addition, one should carefully distinguish the false inversion results from the true sub-3 nm particle concentrations.

8IM.9

Effects of Multiple Scattering by Fresh Soot Aerosols on Open-Path Optical Diagnostics of Atmospheric Plumes.

BRADLEY CONRAD, Matthew Johnson, Jeremy Thornock, *Carleton University*

Combustion-generated soot (often termed black carbon when quantified optically) has been identified as the second-strongest direct radiative forcer in our atmosphere. Globally, soot emission sources include residential combustion, biomass burning, agricultural waste burning, transportation, and gas flaring. Apart from the transportation sector, most soot emissions are from open-atmosphere combustion processes that are inherently difficult to quantify. This has impeded development of accurate global soot emissions inventories. However, non-invasive, open-path optical diagnostics of soot-laden atmospheric plumes are a promising measurement approach that is intrinsically well-suited to this challenge.

Sky-LOSA (i.e. line-of-sight attenuation of skylight) is one example of an open-path optical technique for soot measurement, which has been successfully applied to the measurement of soot emission rate from flares in the oil and gas (OG) industry (e.g. Conrad and Johnson 2017). In this approach, time-resolved grayscale images of a plume are analyzed over a narrow bandwidth in the visible spectrum. The observed transmittance of the soot-laden plume is coupled with two-dimensional velocity data, computed with image correlation velocimetry, to derive the mass emission rate of soot through an artificial control surface in the image plane. The enabling element of the sky-LOSA measurement is the correction of the observed plume transmittance for the in-scattering of skylight and sunlight by the plume, to quantify path-integrated soot concentration at each pixel. In the current algorithm, this is accomplished by assuming only single-scattering of ambient light by the plume. In the limit of an optically thin plume, this is inherently valid; however, as the optical density of the plume increases, interparticle multiple scattering events bias the correction of the observed transmittance for skylight and sunlight.

This work seeks to quantify the effect of multiple scattering by soot on the accuracy and detection limits of open-path optical diagnostics, with a focus on the sky-LOSA technique. Large eddy simulations of gas flares typical of the upstream OG sector are simulated using the massively-parallel ARCHES software under the Uintah computational framework. Gas phase concentration fields of high spatiotemporal resolution are scaled to provide realistic turbulent fields of soot number density. These data are then coupled with calibrations of the sky-LOSA camera under a Reverse Monte Carlo method to assess skylight and sunlight measurement bias by higher-order scattering events. The utility of a multiple scattering correction to Beer-Lambert law is discussed and results are used to infer the relation between multiple scattering effects, plume geometry, and vortex street metrics.

8LC.1

Calibration and Long-Term Performance Evaluation of Low-Cost Sensors for Gas and Fine Particulate Mass Monitoring with RAMPs. CARL MALINGS, Rebecca Tanzer, Provat Saha, Aja Ellis, Rose Eilenberg, Aliaksei Hauryliuk, Sriniwasa Prabhu Nehru Kumar, Naomi Zimmerman, Levent Burak Kara, Albert Presto, R. Subramanian, *Carnegie Mellon University*

Assessing urban air quality and its variability at a high resolution in space and time requires a large network of monitoring sites. The cost of implementing such a network can be prohibitive if traditional high-precision but high-cost reference instruments are used. As an alternative, the Real-time Affordable Multi-Pollutant (RAMP) sensor system has been developed at the Center for Atmospheric Particle Studies of Carnegie Mellon University, in collaboration with SenSevere (Pittsburgh, PA). The RAMP uses electrochemical sensors to measure concentrations of up to four gaseous pollutants out of carbon monoxide (CO), sulfur dioxide (SO_2), nitric oxide (NO), nitrogen dioxide (NO_2), Ozone (O_3), and volatile organic compounds (VOCs), and also includes sensors for temperature and relative humidity. Furthermore, it can interface with external sensors measuring fine particulate matter ($PM_{2.5}$).

Calibration models are developed for each of the electrochemical gas sensors as well as the Met-One Neighborhood Particulate Monitor (NPM) and PurpleAir external PM sensors deployed with the RAMPs. For the electrochemical sensors, cross-sensitivities with other gases as well as temperature and relative humidity impact the responses of the sensors. For the particulate sensors, corrections for aerosol hygroscopic growth at high humidity and local aerosol size distribution relative to sensor detection limits are required.

Various approaches were evaluated to generate calibration models to match raw sensor readings to reference-grade instruments with which the RAMPs were collocated prior to deployment. Data from the collocation are divided into a set used to train models and a separate testing set for validation. Simple linear and quadratic regression were applied, along with multiple nonparametric approaches. A nearest-neighbors clustering algorithm matches new measurements to similar observations in the training data. A neural network uses layers of simple operations to perform complicated nonlinear transformations. A random forest model uses sets of decision rules to group measurements and averages results across these sets. A hybrid random forest model combines random forest and linear models to generalize beyond the training data range. For each approach, separate models were calibrated for each RAMP, and generic models were also created which were applicable across all RAMPs.

Performance of these calibration techniques was assessed in terms of correlation (measured by Pearson correlation coefficient, R) and estimation error (coefficient of variation of the mean absolute error, CvMAE). Simple linear and quadratic models were found to work sufficiently well for CO and O_3 sensors, having comparable performance metrics with more sophisticated nonparametric models (median R above 0.9, median CvMAE below 0.2). For other electrochemical sensors, the hybrid random forest model tended to have the best overall performance. However, performance varied among these sensors, with SO_2 having a relatively low error (median CvMAE 0.34) but also low correlation (median R 0.45), while for NO_2 correlation was relatively better (median R 0.59) but error was worse (median CvMAE 0.47). Compared to RAMP-specific models, general models tended to have comparable performance (average CvMAE increase of 0.1, average R decrease of 0.05).

For the external PM sensors, a correction using RAMP measurements and an average aerosol chemical composition and size for the city of Pittsburgh was applied first. This was followed by additional empirical linear corrections based on collocation with regulatory monitors. Across 12 NPM sensors, median bias was 0.3 $\mu g/m^3$ (range -1.8 to +5.7 $\mu g/m^3$), median mean absolute error was 3.4 $\mu g/m^3$, and median R was 0.93. We shall present results from similar testing of 36 NPM sensor and 12 PurpleAir sensors from such collocations and the performance of the RAMP gas and external $PM_{2.5}$ sensors during long-term (over 12 months) field deployment.

8LC.2

One Year Spatial and Temporal Variability of PM in a Southern California Community using an Air Quality Sensors Network. BRANDON FEENSTRA, Vasileios Papapostolou, Ross Cheung, Andrea Polidori, *South Coast Air Quality Management District*

Technological advances have allowed for governments, academia, communities, and citizen scientists to use new low-cost air quality sensors to measure air pollution at unprecedented spatial and temporal scales. This study presents an analysis of a complete year of measurements from a distributed network of 24 Purple Air PA-II particulate matter (PM) sensors deployed in Southern California at stationary outdoor locations. The PA-II sensor measures PM mass concentrations in three size ranges (PM1.0, PM2.5, and PM10), as well as temperature and relative humidity. A 5-week pilot study was conducted prior to this work to address potential sensor hardware and software issues and was presented elsewhere. The project methodology for sensor selection and evaluation, citizen science deployment, and collocation testing (pre- and post-deployment) will be presented along with lessons learned in community air monitoring. The challenges related to data management and analysis will be discussed with results showing the spatial and temporal variability of aerosols at a neighborhood scale.

8LC.3

Field Validation of a Low-Cost Integrated PM2.5 and Aerosol Optical Depth Monitor. ERIC WENDT, Jessica Tryner, Christian L'Orange, Bonne Ford, Casey Quinn, John Mehaffy, Jeffrey R. Pierce, Shantanu Jathar, Dan Miller-Lionberg, John Volckens, *Colorado State University*

Atmospheric particulate matter smaller than 2.5 microns in diameter ($PM_{2.5}$) impacts public health, the environment, and the climate. Reliable estimates of health and climate impacts require accurate measurements of $PM_{2.5}$ at a global scale. Satellite-based measurements of Aerosol Optical Depth (AOD) may be used to quantify surface-level $PM_{2.5}$ concentrations if the AOD:$PM_{2.5}$ ratio is well constrained. These satellite-based measurements provide estimates of $PM_{2.5}$ concentrations in regions where surface PM2.5 monitors are unavailable, but the AOD:$PM_{2.5}$ ratio used for these predictions is subject to ongoing inquiry. Spatially dense ground-based networks of accurate co-located AOD and $PM_{2.5}$ measurements are necessary to better define the AOD:$PM_{2.5}$ ratio. However, the lack of an integrated $PM_{2.5}$ and AOD monitor combined with the high cost ($10,000 - $45,000) of separate monitors has prevented such a network from being actualized.

We have developed a compact, low-cost (<$850) monitor capable of simultaneous measurement of AOD (at 440, 520, 680 and 870nm), filter-based $PM_{2.5}$ concentration, and real-time $PM_{2.5}$ concentration. The monitor’s small size, durability, low cost, and robust measurement capability circumvent some of the prior barriers to attaining a spatially dense distribution of measurements. Here we present the results of a field validation campaign spanning the latter half of 2017. The campaign consisted of a series of co-location studies where AOD and $PM_{2.5}$ measurements were independently validated relative to reference monitors. The AOD sensors were evaluated against two AOD monitors in the Aerosol Robotics Network (AERONET). A total of 130 concurrent co-located measurements were made at each of the 4 wavelengths. The mean absolute error was 0.0079 AOD units (across all wavelengths), yielding an average relative error of 10%. Filter-based gravimetric sampling capability was evaluated against EPA Federal Reference Methods (FRMs) in a series of 39 paired (48-hr) samples. Average 48 hour concentrations examined ranged from 3.9 to 12.4 ug/m^3. Strong agreement was found between the monitor gravimetric $PM_{2.5}$ and the FRM measurements. The mean absolute error was 0.83 µg/m^3 corresponding with an average relative error of 8%. The real-time sensor included in the monitor was evaluated against a real-time Federal Equivalent Method monitor (GRIMM model EDM 180). Close agreement was observed after real-time measurements were corrected to the filter measurements. These field validation results for this novel monitor demonstrate that AOD and $PM_{2.5}$ can be accurately measured for the evaluation of AOD:$PM_{2.5}$ ratios.

8LC.4

Using an Electrostatic Sensor to Measure Real Time PM Levels in Engine Exhaust. MATTI MARICQ, David Bilby, *Ford Motor Company*

Combustion engines are under pressure to meet increasingly stringent particulate matter emissions standards world wide. For many engine technologies, such as diesel engines, the only way to meet these standards is via exhaust particulate filters. In turn, these devices require on-board diagnostics to ensure their proper function over the full useful life of the vehicle. Identifying a low cost sensor technology capable of robust operation in an engine exhaust pipe is a difficult challenge. The currently used sensors operate by recording a current increase as soot deposits on the sensor element and produces carbon bridges across a pair of electrodes. This technology provides a qualitative means to assess diesel particulate filter (DPF) performance, but as the in-use emissions allowances are brought closer to the regulatory limits they lack the necessary sensitivity and time resolution.

A potential alternative sensor concept is based on a simple electrostatic trap. It is predicated on the intriguing physics of electrically charged soot particles in an electric field. A bipolar electrical charge arises naturally on soot particles as a result of combustion chemistry. As the electric field draws the charged soot agglomerates to the electrodes they grow into elongated dendritic structures normal to the electrode. Above a critical height, these dendrites fragment and carry a large electric field induced charge between the electrodes, easily producing currents of tens of nanoamperes. This current is proportional to the soot concentration; hence, in principle it provides a real time means to monitor soot levels in engine exhaust.

However, this electrostatic sensor responds not just to soot level, but also to the flow rate through the sensor. Flow through the sensor occurs due to the pressure drop across the sensor tip; sensor flow rate changes in response to exhaust pipe flow. The dendrites are not exactly normal to the electrodes; rather they increasingly tilt as a function of sensor flow. Increases in flow rate tilts the dendrites and causes sensor dead time while the dendrites grow to reach their new critical length. Conversely, decreases in flow cause a large spike in current from the release of fragments from the suddenly more upright dendrites.

In spite of this flow induced interference we show that a useful measure of PM emissions can be obtained from the cumulative sensor signal. Namely, the flow effects approximately cancel out over time; the current bursts during flow decreases are compensated by the dead time during flow increases. This talk will present data demonstrating the fragment breakoff mechanism for sensor operation, the flow effects on sensor response and vehicle based comparisons between sensor response and photo-acoustic measurements of soot mass emissions.

8LC.5

New Test Method for the Low Cost Dust Sensors. KANG-HO AHN, Yong-Hee Park, Woo-Young Kim, Hee-Sang Kim, *Hanyang University, R. of Korea*

Why do we need a new test method for the low cost dust sensors?
The low cost dust sensors have widely been used recently for the detection of atmospheric particles. The operating principle of these sensors is based on the light scattering of the particles either by a LED or a Laser light. However, the measurement accuracy of the sensors has always been questioned by many users. Two types of test methods are known for the evaluation of the sensors, i.e., a chamber method and a continuously flowing low speed wind tunnel method with several different types of test particles. A cigarette smoke, Arizona Road Dust, KCl, and many other types of materials have been used for the sensor performance evaluation. In this test method, KCl has been used not only because of the easiness of the size distribution control, but also the easiness of handling. The density and the purity of the KCl are also well defined.

Experimental method
KCl solution is sprayed in order to generate droplets, and then mixed with clean dry air to evaporate droplets. This process will make solid KCl particles. The static charge of the particles will be neutralized by a soft X-ray. These particles are diluted with clean dry air again. And then particles are introduced into the test duct. The cross section of the test duct is a regular quadrilateral. The flow velocity at the test section in the duct should be 0.1 ± 0.05 m/s at all 5 measurement points. The flow velocity measurement points are the centers of the each quadrant of the cross-section of the test duct. In addition, the particle concentration uniformity in the test duct at the 5 sampling points should not exceed ±15% of the mean value of the 5 measurement points. The 5 flow uniformity measurement points are identical to the 5 particle sampling points. The 3 test specimens are place in the test duct with a research grade reference particle counter sampling probe that is inserted into the test duct. And then KCl particle concentration is exponentially decreased as a function of time in the test duct. The low cost dust sensor readings and the reference particle counter data are plotted on a semi-log graph as a function of time. From this test results one can easily figure out not only the dynamic performance of the low cost sensors but also the accuracy of the sensors with very short sensor evaluation time. The sensor test time usually takes less than 10 minutes. More detailed test procedure and some of the test results will be presented at the conference.

8LC.6

Possibilities and Limitations of Low-cost PM Sensors. CHRISTOF ASBACH, Michael Spreitzer, Michael Bässler, Thorsten Schultze, Jörg Lindermann, Heinz Kaminski, Bryan Hellack, Ana Maria Todea, *IUTA, Duisburg, Germany*

The development of low-cost particulate matter (PM) sensors has gained rapid pace in the recent years. These sensors offer numerous new possibilities to both researchers as well as the general public through citizen science activities. As an example, the OK Lab initiative uses Nova Fitness SDS 011 low-cost sensors to measure the spatio-temporal distribution of PM10 and PM2.5. They started in Stuttgart, one of Germany's most polluted cities, but meanwhile the network has extended all over Germany (www.luftdaten.info). The costs for such sensors range from a few Euros/Dollars for simple, photometric sensors to a few hundred Euros/Dollars for size resolving optical spectrometers. Besides their potential use for measuring ambient PM10 or PM2.5 concentrations or indoor or workplace air pollution, they can also be applied in a variety of laboratory based studies in the field of aerosol science. However, in all these applications, several limitations apply that need to be known in order to judge whether or not the use of a low-cost sensor or a sensor network is capable of delivering the desired results. For example, the particle shape and refractive index have to be known or assumed for their calibration. In case of photometric sensors, assumptions regarding the particle size distribution are additionally needed for calibration. If the actual aerosol properties differ from the ones used during calibration, the measurement results will be biased. Temperature and humidity were shown to affect the accuracy of both, photometric sensors and spectrometers.

In order to elucidate their possibilities and limitations, we studied in detail the response of three different sensor types, namely the Sharp Dust Sensor (photometric, approximately 7.50 €/9 US$), Nova Fitness SDS011 (photometric, approximately 15 €/18 US$) and Alphasense OPC-N2 (size resolving spectrometer, approximately 400 €/480 US$). Between three and ten specimens of each sensor type were tested. All sensors have undergone a thorough lab study using a variety of test aerosols, representing a wide range of typical size distributions and refractive indices. A limited number of the sensors were aged with diesel soot in an accelerated aging test, mimicking one year operation at the EU annual PM10 limit value of 40 µg/m^3. The Sharp and SDS 011 were additionally tested in an ambient air quality measurement station in parallel with reference instrumentation.

It was shown that the low cost sensors can in principle deliver reproducible results, but the accuracy, especially of the photometric sensors, strongly depends on the correctness of the assumptions made during the calibration. Furthermore, measurement errors because of changing ambient conditions and aging of the sensors must not be ignored. While these sensors open a wide range of ambient, indoor and laboratory applications of these sensors, care must be taken if they are applied in areas with varying particle properties and/or changing temperature and humidity levels.

The measurements carried out in the laboratory and in the field will be presented and the results discussed in view of the possibilities and limitations of the low-cost sensors.

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8LC.7

Field Calibration of 50 AQMESH Air Quality Sensors. Jacob Swanson, TRES WUERFFEL, Monika Vadali, *Minnesota State University, Mankato*

Understanding small-scale differences in air pollution is essential to minimizing exposure to harmful air pollutants, particularly among vulnerable communities such as communities of concentrated race or poverty. Traditional air monitoring methods are cost-prohibitive to deploy at the level of coverage needed to investigate this important question. However, low-cost sensors that measure air pollutants of concern are now available. The overall objective of this work is to deploy an innovative monitoring approach using low-cost air sensor technology to increase understanding of the variability of air pollutants in urban areas. Data will be used to 1) evaluate pollution reduction opportunities, and to compare with population vulnerability and health outcome data, 2) evaluate the use of new technologies in air pollution sensors as an innovative, cost-effective monitoring strategy, and 3) expand the availability of ambient air quality data to inform decisions, especially regarding public health improvement opportunities.

A network of 50 air quality sensors has been deployed in the St. Paul and Minneapolis neighborhoods, with approximately one sensor per zip code. The “Twin Cities” of Minnesota is a major, seven-county metropolitan area comprising about 3.5 million people. The first step of this deployment was field calibration of the 50 sensors. The air quality sensors were AQMESH pods, version 4.0. These sensors cost about $10,000 each or about $1,000 per metric, which we believe to be in the range of “low-cost” measurement technology. AQMESH measures fine particles ($PM_{1.0}$, $PM_{2.5}$, and PM_{10}) and five gases at ppb levels. Gases measured include ozone (O_3), nitrogen oxides (NO and NO_2), sulfur dioxide (SO_2) and carbon monoxide (CO). Additionally, the sensors measure ambient temperature and relative humidity. Raw data collected from the sensors are centrally processed for cross-sensitivity and other factors that influence response using algorithms proprietary to the manufacturer. All sensors were initially deployed together and contiguous to a Minnesota Pollution Control Agency (MPCA) federal reference method (FRM) monitoring station for “field calibration.” Data from sensors was collected for three weeks during the winter. This presentation reports on 1) the efficacy and limitations of the initial, “factory” calibration settings, 2) inter-sensor comparisons, and 3) comparisons and validation with FRM methods for both gases and particles. Overall, for most gases, the factory calibration provided a “usable” calibration for cases where FRM instruments would not be available. Subsequent calibration with FRM data has the potential to improve accuracy. We conclude by discussing long-term strategies to monitor and address reliability, sensor drift, additional field calibration once the sensors are individually deployed, and the possible degradation of sensor elements due to Minnesota-specific prevailing atmospheric conditions.

8LC.8

Improving Quantification Methods for Long-term (24-36 mo.) Low-cost Air Quality Sensor System Deployments. EBEN CROSS, David Hagan, Leah Williams, Jesse Kroll, John Jayne, *Aerodyne Research, Inc.*

Low-cost air quality sensor systems have developed rapidly over the last few years and offer the opportunity to make multi-pollutant air quality monitoring inexpensive and widespread. However, sensors are often unable to deliver accurate, reliable data over extended periods of time due to a lack of understanding of what parameters impact performance and how best to model this interference. This presentation will describe improved calibration model development for electrochemical sensors measuring CO, NO, NO_2, and O_3 utilizing realistically constrained/accelerated laboratory calibration chamber experiments and long-term (24-month) sensor-to-reference co-location field deployments. Model results from various machine learning techniques will be inter-compared with the goal of identifying a robust calibration approach for ambient air quality monitoring applications.

8LC.9

Assessing Ambient Levels and Personal Exposures in Baltimore: The SEARCH Project. MISTI ZAMORA, Kirsten Koehler, Fulizi Xiong, Drew Gentner, Branko Kerkez, *Johns Hopkins Bloomberg School of Public Health*

The main objective of The SEARCH (Solutions for Energy, AiR, Climate, and Health) Center is to investigate emerging energy transitions in the U.S. and resulting air pollution and health outcomes through state-of-the-science modelling and measurements to characterize factors contributing to emissions, air quality, and health. To accomplish this, we are developing novel online multipollutant monitors (both stationary and portable models) to measure air pollutants and greenhouse gases at a high spatiotemporal resolution. We are particularly focusing on leveraging emerging low-cost technologies. In close collaboration with Yale University, we have developed and deployed three units in downtown Baltimore, Maryland in fall 2017. Currently, the monitors are able to measure particulate matter (e.g., $PM_{2.5}$), ozone (O_3), nitrogen dioxide (NO_2), sulfur dioxide (SO_2), carbon monoxide (CO), methane (CH_4), temperature, and relative humidity, with ongoing modifications to expand to include measurements of NO and CO_2. Using the cellphone 3g data network, we are able to view the data in real time. We will eventually deploy 50 of these monitors at 100 locations over a three-year period.

Preliminary field and laboratory results suggest that the novel monitors are able to reliably measure ambient air pollutants, and the precision between monitors is high. The correlation coefficient of the PM sensors to the EPA reference instrument was 0.95 for measurements collected over several days in downtown Baltimore. Extensive laboratory testing of the PM sensors revealed that the sensors are able to consistently measure a wide range of aerosol sources (e.g., Incense, Oleic Acid, NaCl, Talcum Powder, Ambient Indoor Air, and Cooking Emissions). Further tests have demonstrated that the monitors are able to produce meaningful data in high and low moisture environments and in cold temperatures ($<0\ ^oC$).

8MG.1

Sources and Impacts of Megacities Emissions from Local to Global Scales: Challenges and Opportunities for Mitigation.

LUISA MOLINA, *Molina Center for Energy and Environment*

Urbanization has been a major driver of development and economic progress, but has also created substantial challenges on the natural environment, with impacts at urban, regional and global levels. In recent decades, air pollution has become one of the most important problems of megacities and large urban complexes and has serious consequences on public health, causes urban and regional haze, and has the potential to contribute significantly to climate change. However, as the centers of economic growth, technological advances, social and cultural dynamics, these urban centers also offer opportunities to manage a growing population in a sustainable way. Managing the megacities sustainably will be one of the major challenges in the coming years.

This presentation will give an overview of the current status of studies on the complex interactions between air quality, climate and megacities, and the challenges and opportunities for mitigating the impacts.

8MG.2

Fine Particles Sources in São Paulo: Evolution of Sources Identification for the Last 30 Years. MARIA DE FATIMA ANDRADE, Regina Maura Miranda, Luis Mendes Santos, Yann Marien, *University of Sao Paulo*

Brazil relies on hydroelectricity for more than 75% of its electricity and the transport sector is the main emitter of pollutants from the energy sector. This can be observed mainly in the capital cities of the country where the vehicular emissions are the main source of atmospheric aerosols. Brazil has two metropolitan areas with more than 10 million inhabitants (Sao Paulo and Rio de Janeiro). The Metropolitan Area of Sao Paulo (MASP) is the biggest metropolitan area of the country with more than 21 million inhabitants, corresponding to more than 11% of the total population of the country. The vehicular fleet, composed of more than 7 million units, is responsible for more than 97% of CO, 67.5% of NOx and 79% of HC emissions. The vehicles can run on ethanol, gasohol (gasoline with 25% ethanol) and diesel (or biodiesel). The fine particles (PM2.5) and ozone are the pollutants that present values above the air quality standards in compliance with the Sao Paulo State legislation. In the beginning of the 80´s the evaluation of atmospheric aerosols sources responsibility was mainly based on the application of the so called receptor models: chemical mass balance, factor analysis, principal component analysis and others. In MASP the receptor models started to be applied after initiating the capability of analyzing trace-elements components through x-Ray Fluorescent analysis. The receptor models showed the importance of the industrial sector and vehicular fleet in the 80´s and throughout the years there was a change in the sources impacts on the air quality. The changes were due to variations in economic situation, characteristics of the city evolving from industrialized to tertiary sector (commerce, services) which is now the dominant employer. The implementation of standards for pollutants emission by the vehicular fleet, the establishment of restrictions to the traffic of vehicles in the downtown area and the modification from fuel oil to electricity in the industries changed the drivers of the pollutants emission. Many uncertainties related to the source apportionment were due to the statistical methods. We did a historical analysis of the sources profile evolution comparing those profiles identified through Absolute Principal Component Analysis with Positive Matrix Factorization. To do this we recovered the oldest database available and remodeled the statistical analysis of the data. We observed that V and Ni, used as tracers for burning of fuel in industries, are not well correlated. Meanwhile, P and S, are now very well correlated and can be used as tracers for the mobile source, mainly diesel. We found the presence of these elements at the same ratio at bus terminals and trucks garage. The participation of the mobile source to total PM2.5 has increased from 40-45% in 80´s to 45-60% in 2013-2014. The combination of different receptor models continues to be the best practice to analyze the importance of the sources to the concentration of particulate matter. The air quality has not improved as expected due to the lack of coordination among urban, transport and traffic policies, resulting in more time for commuting in large cities, due to traffic congestion and the increase in the use of private cars.

8MG.3

Spatio-Temporal Trends and Source Apportionment of Fossil Fuel and Biomass Burning Black Carbon (Bc) in the Los Angeles Basin.

AMIRHOSEIN MOUSAVI, Mohammad Sowlat, Sina Hasheminassab, Andrea Polidori, Constantinos Sioutas, *University of Southern California*

In this study, spatio-temporal trends of black carbon (BC) were investigated at four sites, including central Los Angeles (CELA), Anaheim, Fontana, and Riverside (ranging from near-road to sub-urban), in the Los Angeles Basin between 2012-2013 and 2016-2017, and sources of BC were apportioned using the Equivalent Black Carbon (EBC) model. Seven-wavelength Aethalometers (AEE33) were used for BC measurements in this study. BC measurement results revealed that Anaheim had the highest annual total BC concentration (1.37 $\mu g.m^{-3}$) across all sites. Furthermore, BC concentrations in the colder season were approximately twice as high as the levels in the warm season, increasing from 0.60 to 1.17 $\mu g.m^{-3}$, 0.74 to 2.01 $\mu g.m^{-3}$, and 1.24 to 1.33 $\mu g.m^{-3}$, 0.71 to 1.30 $\mu g.m^{-3}$ for CELA, Anaheim, Fontana, and Riverside, respectively. In addition, EBC source apportionment results indicated that the annual fossil fuel combustion contributions to the total BC concentrations (varying between 82% in Riverside to 91% in CELA) are drastically higher than those of biomass burning (varying between 9.3% in CELA to 18.7% in Riverside). In the sites adjacent to major freeways, such as CELA and Anaheim, the aforementioned effect was more pronounced. In addition, the relative contributions of fossil fuel combustion and biomass burning to the total BC concentrations were higher in warm and cold seasons, respectively. For fossil fuel originated Black Carbon (BC_{ff}), major peaks were observed during the traffic rush hours, whereas the contribution of black carbon that originated from biomass burning (BC_{bb}) was maximum in the cold season especially during nighttime, reaching values as high as 25-30% of total BC concentrations. Moreover, due to the implementation of strict regulations in California, BC concentrations and the relative contributions of BC_{ff} to total BC concentrations have gone down since 2012, indicating the efficacy of the regulations that have been put into effect. Based on the main result of the study, due to stricter regulations on controlling fossil fuel combustion sources emissions, BC_{ff} is experiencing a decreasing trend over the years. Consequently, this will increase the relative impact of non-fossil fuel combustion sources, including biomass burning, to the overall BC concentrations.

8MG.4

Source Apportionment of High Resolution Aerosol Trace Elements in Beijing, China. P. RAI, Markus Furger, Jay G. Slowik, Francesco Canonaco, Rujin Huang, Junji Cao, Urs Baltensperger, Andre S.H. Prévôt, *Paul Scherrer Institute*

In the context of rapid economic development and industrial growth in Asian countries, particularly in China, anthropogenic emissions into the atmosphere have had a drastic increase in recent years. Heavily urbanized areas are characterized by a wide array of particle sources, which must be quantified for the formulation of efficient pollution mitigation strategies. Receptor modeling of high resolution data and near real time measurements of trace elements adds greater temporal variabilities to certain source apportionment analyses, which can assist in the identification of local anthropogenic sources such as traffic and industries.

Here we present source apportionment of highly time resolved and near real time measurements of trace metals in Beijing, China during winter time (November/December 2017). During the campaign PM_{10} and $PM_{2.5}$ were sampled with 1-hour time resolution alternatively by an Xact® 625i ambient metals monitor. Sources were resolved using the multilinear engine (ME-2) implementation of positive matrix factorization (Paatero, 1999; Canonaco et al 2013).

The sampling site in Beijing was located in the north of the urban core with two main roads at about 800 m in south and west directions. We found five sources in both size fractions, mineral dust, traffic, S-rich and regional background sources, like industrial and coal combustion, derived from ME-2 analysis. Mineral dust elements (e.g. Al, Si, Ca, Ti, Fe, V) are elevated through the day (2-3 times higher than at night), suggesting their concentrations are driven by resuspension due to anthropogenic activities. While there is no strong diurnal patterns for S-rich, coal combustion and industrial elements (e.g. Cl, Ni, Co, Zn) indicate more diffuse sources. In addition to the sources resolved in both size ranges, we find (size-dependent) evidence for biomass burning and metal smelters emissions. Traffic-related elements (e.g. Cu, Sb, Cr, Ba, Fe, Sn, Zr, Mn) in both size ranges show prominent peaks during the morning and evening rush hours, as is typically the case for traffic-related pollutants similar to NO_x and CO. Both size ranges show distinguish maxima peaks during morning and evening hours. The strong night peak in $PM_{2.5}$ size fraction might be related to truck activity, which is enhanced during the night hours as truck activity is banned during the day. We will discuss source identification, quantification, and contributions to total PM at this sampling site.

Acknowledgements
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Keywords: trace elements, source apportionment, traffic emission, urban aerosol

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8MG.5

Assessment of PM Exposures during Commute in Megacity of Karachi, Pakistan. Kamran Khan, HAIDER KHWAJA, Sumayya Saied, Azhar Siddique, Saiyada Masood, Mirza M. Hussain, *University of Karachi*

Karachi is the largest city of Pakistan, with a population of more than 20 million. The rapid and continuing increase in the population, urbanization, automobiles, and industries combined with climate change and geogenic conditions have resulted in severe ambient air pollution problems in Karachi with serious health impacts. No systematic measurements of air pollution in urban cities of Pakistan have been done until now. To assess the extent of personal exposure and quantification of the particulate matter (PM) concentration, we conducted the first mobile PM monitoring campaign in Karachi. A portable laser-operated aerosol mass analyzer AEROCET 531 was used to record geo-located size-segregated PM mass (TSP, PM_{10}, PM_7, $PM_{2.5}$, and PM_1) concentrations. Seven in-vehicle tracks in different commercial regions of Karachi were studied. All routes are characterized by heavy traffic volumes with a variety of vehicles running with different type of fuels. Maps of routes were generated by using ArcGIS 10.1® software and IDW tool was used to generate the spatial interpolations of the PM. Mean concentrations across the seven tracks were: TSP (685 $\mu g/m^3$), PM_{10} (527 $\mu g/m^3$), PM_7 (386 $\mu g/m^3$), $PM_{2.5}$ (51.9 $\mu g/m^3$), and PM_1 (8.7 $\mu g/m^3$). PM concentrations showed strong spatial variability along each track. High volume of traffic, industries, construction work, and re-suspension of particles all collectively gives rise to high PM concentrations and posing the threatening effect to micro- environment and human health. To tackle the major concern of PM pollution, policy makers must take steps to reduce vehicular emissions, set up mass transit system, and limit industrial pollution.

8MG.6

Submicron Aerosol Composition in the World's Most Polluted Megacity: The Delhi Aerosol Supersite Campaign.

SHAHZAD GANI, Sahil Bhandari, Sarah Seraj, Dongyu S. Wang, Kanan Patel, Prashant Soni, Zainab Arub, Gazala Habib, Lea Hildebrandt Ruiz, Joshua Apte, *University of Texas at Austin*

Delhi is one of the most polluted megacities in the world, where annual average $PM_{2.5}$ levels exceed 130 μg m^{-3}, and wintertime episodic concentrations commonly exceed 500 μg m^{-3}. However, policies to improve air quality and public health are impeded by a limited understanding of the sources and atmospheric dynamics of air pollutants. Here we report on 1.5 years of data from the Delhi Aerosol Supersite. This site, located at Indian Institute of Technology Delhi, is the first long-term chemical characterization of ambient submicron aerosol in India, with near-continuous online measurements of aerosol composition and size distribution since January 2017. Our measurements include non-refractory PM_1 (NR-PM_1, via Aerodyne's aerosol chemical speciation monitor, ACSM), black carbon (BC, via aethalometer) and particle size distributions (scanning mobility particle sizer).

We observe marked seasonal and diurnal variability in the concentration, composition and size distribution of PM_1 owing to the interactions of sources and atmospheric mixing. Winter is the most polluted period of the year with average PM_1 ($NRPM_1$ + BC) mass concentrations of 130 μg m^{-3}. Monsoon was the least polluted with 40 μg m^{-3} and summer, spring and autumn between 50 – 70 μg m^{-3}. Organics are the single-largest PM_1 mass component for all seasons and times of day (~50%). While the average BC concentration was 17 μg m^{-3} for winter and 7 – 13 μg m^{-3} for all other seasons, BC only contributed to 13% of the PM_1 mass concentration in the winter compared to 16 – 22% for the other seasons. We observe average wintertime chloride concentrations of 11 μg m^{-3} (~10% of observed PM_1 mass concentrations). Diurnal cycles of chloride have a pronounced early morning peak, with episodic concentrations exceeding 100 μg m^{-3}, among the highest levels observed anywhere in the world. Sulfate contributes ~ 16 – 19% of PM_1 mass in the warmer months; 9 – 11% for winter and spring, perhaps reflecting more efficient photochemical formation of sulfate during warmer months. Boundary layer height exerts strong influence on diurnal cycles of all primary pollutants, with nocturnal concentrations of primary species routinely exceeding daytime levels by 3-5×.

While the wintertime mass concentrations were 4-5× times higher than during the cleaner monsoon months, the average number concentrations were only 1.9× higher during wintertime compared to monsoon (37,000 # cm^{-3} vs. 20,000 # cm^{-3}). We attribute this relatively low enhancement in wintertime particle number concentration to coagulative scavenging. Concurrently, coagulation leads to a strongly pronounced accumulation mode in particle size distributions, with unusually large count median diameters during polluted conditions (~90-130 nm).

Positive matrix factorization (PMF) conducted on the ACSM mass spectra provides further information on the sources and atmospheric processes that affect NR-PM_1 levels in Delhi. Hydrocarbon-like organic aerosol (HOA) exhibits strong diurnal variability, reflecting the impact of primary combustion emissions modulated by diurnal cycles in mixing height. As observed in other megacities, oxidized organic aerosol (OOA) is the largest constituent of the organic aerosol throughout the year, demonstrating the profound influence of secondary formation on particle concentrations in Delhi. Biomass burning organic aerosol (BBOA) constituted majority of the organic aerosol during extreme wintertime biomass burning events, but was almost absent during the less polluted monsoon months.

Overall, these findings point to the important effects of both primary emissions and regional atmospheric chemistry on influencing the extreme particle concentrations that impact the Delhi megacity region. Future air quality strategies considering Delhi's situation in a regional context will be more effective than policies targeting only local, primary air pollutants.

8MG.7

On Particle-Bound Polycyclic Aromatic Hydrocarbons (PPAH) and Links to Gaseous Emissions in Mexico City. LUIS ANTONIO LADINO, Graciela Raga, Darrel Baumgardner, *Universidad Nacional Autónoma de México, Mexico City, Mexico*

Mexico City is a densely populated megacity with average PM10 and PM2.5 levels frequently above those indicated as health threatening for humans by the World Health Organization. Polycyclic aromatic hydrocarbons (PAH) can be emitted by anthropogenic sources as the result of the incomplete combustion of organic matter and fossil fuels and they represent an important risk for human health under poor air quality conditions. High concentrations of PAHs have been linked with cancer and other respiratory diseases. Although particle-bound PAHs (PPAHs) have been previously studied in Mexico City, their temporal scales are not fully understood given the short sampling periods (up to five weeks) during which they were evaluated.

Recent, automated and continuous measurements of PPAH concentration made in Mexico City during one full year (April, 2016 to March, 2017) show average PPAH concentration of 31.7±29.9 ng m^{-3} at the sampling location. The highest concentrations were observed in winter. On a daily basis, the maximum concentrations were observed between 6:00 and 11:00 am, as high as 352 ng m^{-3}. The average PPAHs levels measured in spring 2016 were found to be ca. 50% higher than those that were previously measured in spring 2003, in approximately the same location. Given the lack of instrumentation to measure PPAH at most air quality monitoring stations, a proxy was developed based upon the concentrations of carbon monoxide (CO) and nitrous oxides (NOx), which are typically measured at urban monitoring stations worldwide. Such parametrizations suggest that people living in the North and Northeast of Mexico City are at higher risk to develop respiratory problems given that in these locations the PPAH concentrations are expected to be higher than in the rest of the city.

8MG.8

Chemical Composition of Ambient PM2.5 and PM10 for an Industrial City, Ghaziabad, India. LOVLEEN GUPTA, Ramya Sunder Raman, Gazala Habib, *IIT Delhi*

Ghaziabad is an industrial and semi-urban city sharing border on one side with New Delhi, Indian national capital. Several articles in the Indian and International press have termed Ghaziabad as the most polluted city in India. The 24 hour average $PM_{2.5}$ and PM_{10} concentrations reported[1] in Ghaziabad during April 2017[2] - Dec 2017 were 145.35 (±132.9) $\mu g/m^3$ and 298.15 (±183.98) $\mu g/m^3$, respectively. During this period, $PM_{2.5}$ and PM_{10} maxima were as high as 752.19 $\mu g/m^3$ and 949.71 $\mu g/m^3$, respectively. These PM concentrations are way above the Indian National Ambient Air Quality Standard (NAAQS) which is 60 $\mu g/m^3$ for $PM_{2.5}$ and 100 $\mu g/m^3$ for PM_{10} (24 hour average). Further, daily average PM concentrations were always above the standards except during the monsoon period (June – August).

Ambient PM concentrations are routinely monitored in India. However, the measurements are often limited to the total mass concentrations of PM_{10} and $PM_{2.5}$. Information on the chemical composition of aerosol particles, essential for developing remediation strategies to prevent further deterioration of local air quality and health of residents of the city are very scarce. Few studies reporting the chemical composition of aerosols in India, focused on the urban areas (metro cities like Delhi, Mumbai, Kolkata, Hyderabad, Chennai). There are hardly any studies over semi-urban and rural areas. Further, no such study has been carried out for Ghaziabad so far.

This study aims to understand the chemical composition of $PM_{2.5}$ and PM_{10} in Ghaziabad. The study will present preliminary results on the ambient concentrations of Organic and Elemental Carbon (OC and EC), water soluble ions and trace elements for the pre-monsoon season (March – May 2018). The PM samples will be collected at two sites in Ghaziabad using ABC-3000 samplers from URG Corporation, USA. The selected sites are located in the upwind and downwind directions of Ghaziabad city. 24 hour integrated PM samples will be collected on Quartz, Nylon and Teflon filters every third day The quartz filters will be subjected to thermal optical analysis for EC and OC, while ions and trace elements will be determined on Nylon and Teflon filters using Ion Chromatography (IC) and Energy Dispersive X-Ray Fluorescence (ED-XRF), respectively. In addition, on-site meteorological parameters (like temperature, Relative Humidity, Wind speed and direction) will also be recorded at both the sites, to assess the influence of meteorology on the chemical constituents of the aerosol and to assess the formation of secondary aerosols.

Acknowledgement:
We thank Uttar Pradesh Pollution Control Board (UPPCB, http://www.uppcb.com/) for funding this work.

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8MG.9

Aerosol Fluxes above Beijing. EIKO NEMITZ, Ben Langford, Chiara Di Marco, Neil Mullinger, Yele Sun, Jian Zhao, Pingqing Fu, *Centre for Ecology and Hydrology*

As part of the UK-China collaborative research programme “Air Pollution and Human Health in a Chinese Megacity”, aerosol fluxes were measured during two contrasting periods in Nov/Dec 2016 and May/June 2017, using the micrometeorological eddy-covariance (EC) flux measurement technique. A fast response ultrasonic anemometer and a total of three particle counters were operated at a height of 102 m on the 325 m meteorological tower at the Institute for Atmospheric Physics (IAP) of the Chinese Academy of Sciences. These included a water-based condensation particle counter (CPC3785, TSI Inc.), and a combination of an Ultra High Sensitive Aerosol Spectrometer (UHSAS, DMT) and Aerodynamic Particle Sizer (APS3321, TSI Inc), together providing size-segregated particle fluxes over the size range 60 nm to 20 µm. Moreover, a sample inlet brought air to a measurement container at the foot of the tower, where an Aerosol Mass Spectrometer (HR-ToF-AMS; Aerodyne Research Inc) and Single Particle Soot Photometer (SP2, DMT) provided a fast response measurement of aerosol chemical composition, suitable for flux calculations of non-refractory NH_4^+, NO_3^-, SO_4^{2-}, Cl^- and organic aerosol in PM_1, as well as black carbon. The AMS total organic aerosol flux was further decomposed by application of Positive Matrix Factorisation to virtual eddy-accumulation data, which was derived from the EC data.

Chemically speciated fluxes were dominated by organic carbon. During winter, both SO_4^{2-} and Cl^- showed emission, most likely from coal combustion, which was absent in summer. NO_3^- and NH_4^+ were emitted in winter, but downward fluxes were observed during summer, which reflects evaporation of NH_4NO_3 in the urban surface layer, below the measurement height. As a consequence the size-segregated particle fluxes were bi-directional during summer daytime conditions, downward fluxes were observed in the accumulation mode (> 0.22 µm) at the same time as the smaller particles were emitted. The PMF results indicated that inner urban organic aerosol emissions were very much dominated by cooking organic aerosol, with further contributions from fossil fuel combustion, whilst secondary organic aerosol components showed little flux. This is in stark contrast to the composition of the concentration, which was dominated by secondary organic aerosol components that must have originated from more regional emissions.

Compared with cooking aerosol emissions, local fossil fuel emissions were quite small, in particular in summer, possibly reflecting the fact that diesel-powered HGV are banned from Beijing during the day. This would suggest that controlling sources such as cooking may have more potential in reducing urban exposure than further control of tail pipe emissions.

9AC.1

Liquid-Liquid Phase Separation in Organic Aerosol Particles Investigated by Environmental X-Ray Microscopy. Jan-David Förster, Christopher Pöhlker, Haijie Tong, Markus Ammann, Florian Ditas, Jörg Raabe, Ulrich Pöschl, David Walter, Benjamin Watts, MEINRAT O. ANDREAE, *Max Planck Institute for Chemistry*

Atmospheric aerosol particles play important roles in the atmosphere and climate system by scattering and absorbing solar radiation and affecting cloud properties. The atmospheric life cycle and climate impacts of aerosol particles largely depend on their phase and mixing state and, particularly, on their hygroscopic response under variable relative humidity. A systematic understanding of the aerosol's dynamic evolution under variable atmospheric conditions is crucial to estimate their overall impact on the atmosphere.
Advanced micro-spectroscopy, especially scanning transmission x-ray microscopy with near-edge x-ray absorption fine structure spectroscopy (STXM-NEXAFS), is a suitable technique to address these dynamic processes with high spatial and chemical resolution.

Humidity variations in the atmosphere can change the morphology and mixing state of aerosol particles substantially [1]. In order to mimic atmospheric aerosol processing and particularly humidity cycling, we built an environmental cell for STXM-NEXAFS, which allows to control temperature, humidity, and pressure in the cell precisely and reliably. STXM-NEXAFS further allows to conduct a chemical characterization of the separated phases.

Here we present results on the observation of liquid-liquid phase separation in laboratory generated secondary organic aerosol particles along the lines of recent studies [2]. Our results show a miscibility gap of the SOA/water system above ~95 % for certain SOA types down to submicron particle sizes. STXM-NEXAFS further allows to conduct a chemical characterization of the separated phases.

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9AC.2

Connecting Phase Separations in Ambient Secondary Organic Aerosol and Ammonium Sulfate Particles to Relative Humidity and Temperature. ANDREW AULT, Amy Bondy, Sydney Niles, Peter Peterson, Little Josie, Rashad Pace, Ryan Moffet, Rachel O'Brien, Bingbing Wang, Alexander Laskin, *University of Michigan*

Secondary organic aerosol (SOA) is a ubiquitous component of submicron ambient aerosol, but its formation mechanisms and the connection between chemical composition and physical properties are not well understood. In recent years, phase has been shown to range from to solid to semi-solid to liquid for ambient particles via bounce measurements, while modeling has predicted that organics should be solid or semi-solid over land. Morphology (e.g. core-shell) of SOA has been primarily studied to the laboratory, where studies have shown morphologies ranging from well-mixed liquid particles to core shell or more complex morphologies as a function of relative humidity (RH) and temperature. However, direct evidence of non-liquid phases and phase separation in individual, ambient particles is limited. Herein, we show that internally mixed SOA and inorganic salt (e.g. ammonium sulfate) particles frequently adopt core-shell or more complex internal structures, likely due to viscous organic components. Ambient morphology is shown to be strongly dependent on the size, as well as contributions from chemical composition and the relative humidity and temperature history of a particle. This has important implications for heterogeneous reactions as organic coatings can inhibit uptake of SOA precursors and the aqueous portion of phase-separated particles is likely to have very different properties (e.g. acidity or ionic strength) than a well-mixed particle with the same composition. It is likely that core-shell or complex structures are prevalent over land and that they play an important role in SOA formation and properties.

9AC.3

Measurements of Acid and Organic Partitioning between Phase-separated SOA/Aqueous Phases. BENJAMIN DEMING, Paul Ziemann, *University of Colorado*

Measurements of aerosol pH vary, but they are typically very acidic, with values as low as 1 not being uncommon. This has important implications for the composition of organic aerosol, which can be influenced by particle-phase reactions involving acid catalysis. For example, alcohols may be converted to alkenes, which are highly reactive towards ozonolysis, and oligomers can be formed through accretion reactions. However, many aerosols are phase-separated, with distinct organic and aqueous portions. There is therefore some question as to the amount of acid an organic species may be exposed to. The purpose of this work is to determine the distribution of acid and SOA components within a model phase-separated system. To this end, we have generated SOA via the reaction of α-pinene with ozone in an environmental chamber and collected filter samples for offline analyses. This reaction has been well characterized by our group and others, and has the added benefit of allowing for the easy formation of milligram quantities of SOA. Partitioning of the SOA was measured directly by mixing it with a chosen aqueous phase and optionally additional organic material, separating the two phases, evaporating the solvents, and weighing with a microbalance. The phase preferences for compounds containing carboxyl, carbonyl, hydroxyl, peroxide, and ester groups was also determined using derivatization-spectrophotometric methods we developed previously for microscale analysis of complex organic aerosol. The partitioning of acid between the two phases was measured by acidifying the two-phase model system, separating the two phases, and precipitating the acid out of the organic phase by the addition of ammonia. The solvent was then evaporated and the residual ammonium sulfate salt weighed using a sensitive microbalance. The organic phases used included SOA formed from α-pinene ozonolysis, and a suite of commercially available solvents that included 2-butanone, ethyl acetate, and propylene carbonate, which span the O/C ratios commonly measured for atmospheric aerosols. The aqueous phase consisted of either pure water or an ammonium sulfate solution, also typical of ambient aerosols. These measurements were then used to derive distribution coefficients for both acid and SOA in phase-separated aerosol. The results from this work will have important implications for the viability of acid-catalyzed mechanisms in models of SOA production.

9AC.4

Uptake of Dicarboxylic Acid Molecules by α-Pinene Secondary Organic Material and Implications for the Role of Particle Phase State and Relative Humidity.

YUEMEI HAN, Jianhuai Ye, Zhaoheng Gong, Pengfei Liu, Suzane de Sá, Karena McKinney, Scot T. Martin, *Harvard University*

Secondary organic material (SOM) particles can exhibit different phase states in amorphous solid, semisolid, and liquid depending on a variety of factors such as relative humidity (RH), temperature, and the reaction history of precursor hydrocarbons. Increasing relative humidity lowers the viscosity of SOM particle and thereby improves their potential for dynamic exchange and reactivity with gas-phase molecules. Given that large amounts of gas-phase organic species are present in the real atmosphere, however, the influence of particle phase state and relative humidity on the uptake of those organic molecules by SOM particles remains poorly understood. This study investigates the uptake of gas-phase dicarboxylic acid molecules at variable RH conditions by atmospherically relevant SOM particles generated from dark ozonolysis of α-pinene. ^{13}C-labeled dicarboxylic acids were applied as probe molecules for quantifying the amount of uptake with aerosol mass spectrometry. A continuously increased uptake of ^{13}C-labeled oxalic, malonic, and α-ketoglutaric acids by α-pinene SOM particles were observed with increasing RH while a saturation of uptake was not reached for RH up to 80%. The studied dicarboxylic acid molecules were possibly well-miscible with α-pinene SOM particles, as indicated from their similar ranges in terms of Hansen Solubility Parameters, an approach used to predict the miscibility of organic materials. A higher uptake amount was obtained as the increase of gas-phase concentration and the decrease of volatility, suggesting these are important factors governing the uptake of the dicarboxylic acid molecules.

9AC.5

The Effects of Aerosol-Phase State and Chemical Composition on Multiphase Chemistry Leading to Isoprene-Derived Secondary Organic Aerosol Formation. YUE ZHANG, Yuzhi Chen, Andrew Lambe, Nicole Olson, Ziying Lei, Rebecca Craig, Manjula Canagaratna, Jordan Krechmer, Zhenfa Zhang, Avram Gold, Timothy Onasch, John Jayne, Douglas Worsnop, Cassandra Gaston, Joel A. Thornton, William Vizuete, Andrew Ault, Jason Surratt, *Boston College; Aerodyne Research, Inc.*

Acid-catalyzed reactions between gas- and particle-phase constituents are an important formation mechanism for atmospheric secondary organic aerosol (SOA). Aerosol phase state, governed by aerosol composition, relative humidity (RH), and temperature, influences the reactive uptake process of gas-phase precursors by altering diffusion rates within particles. However, there is little experimental evidence to show the dependence of reactive uptake processes on particle-phase state with respect to these factors. This laboratory study systematically examines the reactive uptake probability of isoprene-derived epoxydiols (IEPOX) onto acidic ammonium sulfate particles with various types of pre-existing SOA coatings by coupling a flow tube reactor with an iodide-adduct high-resolution time-of-flight chemical ionization mass spectrometer (HR-ToF-CIMS). A uniform layer of organics is coated onto the acidic sulfate particles using the potential aerosol mass (PAM) oxidation flow reactor, confirmed via atomic force microscopy (AFM) and scanning electron microscopy (SEM). The measured reactive uptake probability is parameterized as a function of SOA coating thickness, oxidation state, and RH. Results show that certain pre-existing SOA coatings could significantly reduce the reactive uptake probability of IEPOX, in some cases by nearly an order of magnitude when the coating thickness is only 10 nm.

Particle composition is also analyzed by both online and offline analytical techniques, including an aerosol chemical speciation monitor (ACSM), ultra-performance liquid chromatography interfaced to electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (UPLC/ESI-HR-QTOFMS), and ESI coupled to ion mobility spectrometry high-resolution time-of-flight mass spectrometry (ESI-IMS-HR-TOFMS). Results show that the oxidation state and composition (such as the oligomer content) of aerosol particles jointly contribute to their phase state, thereby altering the diffusion rate of IEPOX in the organic coating and the measured reactive uptake coefficient.

A box model combining experimental data with ambient measurements from the 2013 SOAS campaign is used to assess the effects of pre-existing organic coating on IEPOX-derived SOA formation. The diurnal trend of isoprene-derived SOA mass concentrations with and without coating effects is derived by modeling the experimental uptake coefficient with field-measured data from the southeastern U.S. IEPOX-derived SOA is estimated to be reduced by 16-27% due to pre-existing organic coatings during the afternoon (12-7 PM, local time), corresponding to its highest production period. Our study provides a potential explanation for the discrepancy between model predictions and field measurements of IEPOX-derived SOA reported by previous studies.

Our results suggest that the inorganic and organic components of aerosol particles, as well as their physical and chemical properties, jointly impact the formation, evolution, and fate of ambient SOA. For instance, pre-existing SOA constituents formed from the condensation of semi-volatile species, with certain compositions and phase states, can adversely affect the reactive uptake of gases leading to the formation of additional SOA. These results can be used to accurately characterize the formation and evolution of IEPOX-derived SOA. Moreover, the approach used in this study could be more widely applied to other multiphase chemical systems in regional and global scale models to better predict the impact of SOA on climate, human health, and visibility.

9AC.6

Refining Equilibrium Partitioning: Detailed Chemical Composition, Viscosity and Diffusion Measurements. KELLY PEREIRA, Alfie Mayhew, Grazia Rovelli, Young-Chul Song, Aleksandra Marsh, Stephen Ingram, Simon O'Meara, David Topping, Jonathan P. Reid, Jacqueline F. Hamilton, *University of York*

Secondary organic aerosol (SOA) constitutes a considerable proportion of ambient particulate matter and exhibits substantial chemical complexity. Equilibrium partitioning is a fundamental theorem governing the growth and loss of SOA. However, recent literature has suggested that gas-particle partitioning may be kinetically limited, preventing volatilisation from the SOA due to the physical state of the particle (*e.g.* viscous, glassy). To predict the properties and impacts of SOA in the atmosphere, the processes controlling non-equilibration must be known. This work combines several key components to investigate the effect of the physical state of the SOA on equilibrium partitioning, including detailed chemical speciation and bulk compositional measurements, single particle viscosity/diffusion measurements and modelled simulations for the refinement of predictive tools for multicomponent mixtures.

Experiments were performed in a 300L in-house built continuous flow reactor. Over 50 experiments were performed, investigating SOA formation from the photo-oxidation of α-pinene, β-caryophyllene, limonene and toluene under varying %RH, NO_x and VOC mixing ratios. SOA mass was collected using an electrical low pressure impactor, minimising potential artefacts associated with conventional filter extraction methods. SOA composition was investigated using a variety of state-of-the-art techniques, including ultra-high performance liquid chromatography ultra-high resolution mass spectrometry, ^{1}H and two-dimensional ^{1}H-^{13}C heteronuclear single quantum correlation (HSQC) nuclear magnetic resonance spectroscopy, Fourier transform infra-red spectroscopy and CHNS elemental analysis. High performance liquid chromatography ion trap mass spectrometry coupled to an automated fraction collector was also used for the isolation and collection of individual compounds in α-pinene SOA, providing authentic standards for quantification. Up to 40% of the generated α-pinene SOA mass (by weight) has been quantified, with a range of 3 to 40% depending on experimental conditions (*e.g.* with/without NO_x). Bulk compositional techniques indicate subtle changes in the functionality of the SOA with varying %RH and NO_x mixing ratios, which has little impact on bulk SOA metrics such as average carbon oxidation state. In contrast, individual α-pinene SOA species displayed marked differences in their concentrations during the same experiments. This suggests that the metrics that describe bulk SOA properties are rather insensitive to molecular levels changes, possibly as a result of the production of similar functionalities under varying chamber conditions. Detailed compositional data combined with viscosity and diffusion measurements has the potential to lead to considerable advances in our understanding of the dynamic mechanisms controlling equilibrium partitioning. To our knowledge, this is first study which has combined both detailed chemical composition, viscosity/diffusion measurements and multicomponent model simulations.

9AC.7

Chemical Composition and Implications for Viscosity of SOA at Low Temperature. CLAUDIA MOHR, Wei Huang, Cheng Wu, Yvette Gramlich, Harald Saathoff, Aki Pajunoja, Annele Virtanen, *Stockholm University*

Secondary organic aerosols (SOA) can be transported to or formed in the upper troposphere. Temperature and relative humidity conditions representative of the upper troposphere, however, are rarely simulated in chamber studies, despite their potential importance for the phase state, morphology and chemical composition of SOA particles and thus their cloud formation potential. In the present work, we investigate the chemical composition and viscosity of SOA from α-pinene and toluene formed at conditions corresponding to temperatures of 223 K to 296 K and relative humidities between

We conducted two types of chamber experiments at the AIDA facility at KIT. In most experiments, SOA was directly formed in the dark AIDA chamber kept at different temperatures by reaction of precursors with O_3 or OH radicals. For the second type, SOA from α-pinene was first produced in an adjacent, smaller chamber kept at ambient temperature, and then introduced into the AIDA chamber, kept at different temperatures, where for a subset of experiments it was mixed with the SOA produced from toluene. For about half of the experiments, NO_x was added to investigate its influence on oxidation products and SOA yield. The chemical composition of SOA particles was analyzed with a chemical ionization mass spectrometer with filter inlet for gases and aerosols (FIGAERO-CIMS), deploying iodide as reagent ion.

Comparisons of particle-phase mass spectra for SOA from the oxidation of mixtures of toluene and α-pinene by OH radicals at three different temperatures indicate that the temperature has a significant impact on the chemical composition for these mixed SOA. Mixing particles from α-pinene and toluene oxidation after separated formation does not seem to drastically change the nature of the organic compounds. This is a somewhat expected result, as the time scales of particle mixing and potential subsequent chemical reaction between particle-phase compounds likely lie beyond the time scales of our few-hour-experiments. However, when gaseous compounds of the two precursors are already mixed during the oxidation process before particle formation takes place, different compounds exhibit high signal. In the presence of NO_x, a clear reduction of the SOA yield was observed, especially for compounds with higher masses.

We also present detailed investigations of the shape of signal resulting from the thermal desorption of SOA particles deposited on the Teflon filter in the FIGAERO (thermograms). Single mode thermograms with signal maxima occurring at distinct desorption temperatures (T_{max}) are correlated with a compound's enthalpy of sublimation. Significantly higher T_{max} were observed in the sum thermograms for $C_xH_yO_z$ compounds of α-pinene SOA formed at cold and dry conditions compared to humid and/or warm conditions. The results suggest differences in the viscosity of the formed SOA particles depending on experimental conditions, potentially resulting from high molecular weight organics and/or oligomers. Mass spectra comparison for these conditions support this conclusion.

The results provide insights into the influence of changing temperature and humidity conditions on chemical composition and viscosity of anthropogenic and biogenic SOA during its formation and evolution in the atmosphere.

9AC.8

Secondary Organic Aerosol (SOA) Phase State-Relevant Properties: Evaluation of Impacts in the Southern Great Plains Using CMAQ. ANNMARIE CARLTON, Ying Li, Manabu Shiraiwa, James Smith, Sergey Nizkorodov, Marc Carreras-Sospedra, Donald Dabdub, *University of California, Irvine*

Secondary organic aerosol (SOA) is a dominant contributor to the atmospheric particle matter burden. Historically, atmospheric models struggle to accurately reproduce field measurements of SOA surrogates. Discrepancies may arise from model approaches that describe gas-to-particle partitioning for SOA formation with two assumptions: instantaneous thermodynamic equilibrium, and all organic material is equally miscible. Recent laboratory and field evidence indicates these assumptions are not always valid, in part due to kinetic limitations on partitioning imposed by SOA phase state. SOA transitions between amorphous and semi-solid states as a function of chemical composition, relative humidity and temperature. We calculate the glass transition temperature (Tg), hygroscopicity parameter (κ), and the Gordon-Taylor constant for SOA predicted with the Community Multiscale Air Quality (CMAQ) model and investigate impacts on SOA viscosity. We focus on predictions at the Department of Energy (DOE) monitoring site in the Southern Great Plains in Oklahoma, a location that provides robust chemical climatology for particle properties relevant to SOA phase state. We also compare CMAQ predictions for the intensive observing period during the Holistic Interaction of Shallow Clouds, Aerosols, and Land-Ecosystems (HI-SCALE) field campaign in 2016.

9AM.1

Estimation of Human Exposure to Near Road Emission Sources Using a Hybrid Modeling Framework. Fatema Parvez, KRISTINA WAGSTROM, *University of Connecticut*

Traffic related air pollution is considered one of the major challenges for a large number of urban population. The rapid growth of the world's motor-vehicle fleet due to population growth and economic improvement causes a significant negative impact on public health. As pollutants from roadway emission sources reach background concentration levels within a few hundred meters from the source, it is very challenging to implement a model that captures this behavior. Currently available air quality modeling approaches can compute the source specific pollutant fate on either a regional or a local scale but still lack effective ways to estimate the combined regional and local source contributions to exposure. Temporal variabilities in human activities and differences in pollutant dispersion pattern in stable and unstable atmospheric conditions greatly influence the exposure. Estimating air pollution exposure from local sources such as motor vehicles while considering all the variables impacting the dispersion make the process computationally intensive.

In this study, we develop a hybrid modeling framework combining a regional model, CAMx - Comprehensive Air Quality Model with Extensions, and a local scale dispersion model, RLINE, to estimate concentrations of both primary and secondary species from roadway emission sources. We utilize all chemical and physical processes available in CAMx and use the Particulate Matter Source Apportionment Technology (PSAT) to quantify the concentrations from onroad and non-road emission sources. We employ RLINE to estimate pollutant distribution from onroad emission sources at a finer resolution. Combining these two models, we estimate combined concentrations at a finer spatial resolution and at hourly temporal resolution.

We further conduct an operational model evaluation of our hybrid modeling framework for the year 2011 for NO_2 using both satellite data and regression model data at census block resolution. We find that our hybrid modeling framework performs well with a mean fractional bias 0.15 and a mean fractional error 0.4 when compared to the land-use regression model. We have applied this modeling framework to three major cities in Connecticut (Hartford, New Haven, and Windham) and quantified human exposure to NO_x, $PM_{2.5}$, and elemental carbon (EC). We quantify exposure considering census tract population density and temporal and spatial variability in concentrations. Our approach using a dispersion model is unique as it uses the mass fraction of the total dispersed pollutant at different receptor points and hence is not dependent on extensive roadway emissions data or extensive model runs. Overall, this modeling approach overcomes two major challenges facing hybrid modeling for near roadway exposures - double counting emissions and a lack of temporal variability in estimating concentrations.

9AM.2

Dynamic Health Risk Mapping and Predictive Modelling of the Impact of Metereological Fluctuations on Air Pollution in Yangtze River Delta. JIE YANG, *University of Nottingham Ningbo China*

Overestimating and underestimating the impact of air pollution on the disease burden in the Yangtze River Delta (YRD) may lead to either economic growth being unnecessarily hindered or cardiorespiratory diseases induced by ambient air pollution imposing a huge strain on the national or regional health and insurance system in order to treat the related symptoms. Accurate estimation is thus essential to enable Governmental departments and health officials to implement the most effective measures for dealing with air pollution. Existing models that are employed to estimate the disease burden attributable to ambient air pollution exposure do not properly consider the influence of fluctuating weather patterns on dynamically dispersing or concentrating local sources of air pollution.

This study proposes the use of a novel spatial-temporal mathematical model based on a reaction-diffusion system with time delays to describe the change in relative risk of being exposed to certain particulate matter, which is dependent on both geographical location and its corresponding metereological conditions such as temperature, humidity and wind speed. The model takes into account information about levels of particulate matter (PM) less than 2.5 microns in aerodynamic diameter ($PM_{2.5}$), PM less than 10 microns in aerodynamic diameter (PM_{10}), nitrogen dioxide (NO_2), sulphur dioxide (SO_2), carbon monoxide (CO), ozone (O_3) and also factors in meteorological fluctuations to generate regional dynamic health risk maps in YRD caused by air pollution, focusing on Ningbo city and its surrounding areas as a case study. The simulation results of this model that employs air quality, weather and health data can be used to make predictions about the impact of air pollution on disease burden. It is expected that the results derived from the model may then be used by health officials to make informed decisions about the optimal allocation of limited and valuable resources for reducing the air pollution levels related to those geographical areas of particular concern.

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9AM.3

Modelling the Effects of Natural and Anthropogenic Sources of Aerosols on Weather. PAUL MAKAR, Wanmin Gong, Craig A. Stroud, Ayodeji Akingunola, Balbir Pabla, Jack Chen, Radenko Pavlovic, Michael Moran, Chris McLinden, Junhua Zhang, Jason Milbrandt, David Sills, Katherine Hayden, Shao-Meng Li, Philip Cheung, Qiong Zheng, *Environment and Climate Change Canada*

The “fully coupled” configuration of the Global Environmental Multiscale – Modelling Air-quality and CHemistry (GEM-MACH) chemical weather model was used with two nested grids to examine the relative impacts of anthropogenic versus natural sources of atmospheric particles on weather across North America (outer grid), and in particular the Canadian provinces of Alberta and Saskatchewan (inner grid). This model configuration employs a 12-bin sectional approach for representing the aerosol size distribution, and incorporates direct-effect feedbacks using a Mie scattering approach. Indirect-effect feedbacks are represented through the cloud microphysics’ cloud droplet nucleation process making use of the model-generated particle properties, the resulting cloud droplet distribution influencing radiative transfer and in-cloud particle scavenging, and the resulting precipitation rate influencing below-cloud particle removal. Both the North American 10-km horizontal grid spacing simulations, and the Alberta + Saskatchewan 2.5-km horizontal grid spacing simulations made use of these direct and indirect effect parameterizations.

Five sets of simulations were carried out for the 5-week period June 1st through July 6th, 2018: (1) a “no-feedback/all emissions” simulation, in which the direct and indirect effects of feedbacks were disabled; and emissions include biogenic, anthropogenic, and forest fire sources; (2) a “feedbacks, all emissions” simulation wherein the feedbacks were enabled; (3) a “feedbacks, no anthropogenic emissions” simulation; (4) a “feedbacks, no biogenic emissions” simulation; and (5) a “feedbacks, no forest fire emissions” simulation. Differences between the predictions of these simulations for 2-m and 3-D temperature, 10m and 3D winds, total cloud liquid water content, and surface precipitation were used to show the incremental and relative impacts of anthropogenic, biogenic and forest fire emissions on weather, for both North America the highest resolution nest over Alberta and Saskatchewan. Comparisons will be shown between each model simulation and the available meteorological and air-quality observation data to demonstrate their relative forecast skill.

Each of the 24-hour simulations were initialized from 10-km horizontal grid spacing meteorological analyses updated daily – and hence the resulting variations in the predicted weather examined here describe the relatively short-term impacts on the resulting forecasts. However, these impacts were found to be significant, particularly near large local sources of anthropogenic and forest fire emissions, but also over the larger region of Alberta and Saskatchewan.

9AM.4

Forecasting Smoke Transport and Its Impact on Weather in High-Resolution (3km) HRRR-Smoke Model over the US.

RAVAN AHMADOV, Eric James, Georg Grell, Curtis Alexander, Steven Albers, Ivan Csiszar, Marina Tsidulko, Rick Graw, Stuart McKeen, Shobha Kondragunta, Gabriel Pereira, Brad Pierce, Saulo Freitas, *CU CIRES- NOAA ESRL*

We present a new smoke modeling system, the High-Resolution Rapid Refresh with smoke (HRRR-Smoke) to simulate biomass burning (BB) emissions, plume rise and smoke transport in real time. The HRRR model (without smoke) is run operationally at the National Weather Service with 3km spacing for numerical weather prediction (NWP) over the contiguous US. One of the novelties of this model is the use of the double moment aerosol aware microphysics scheme. This scheme enables a computationally efficient coupling between smoke and model meteorology. HRRR-Smoke simulates fine particulate matter (PM2.5 or smoke) emitted by wildfires and prescribed burns. The model ingests fire radiative power data from various satellite sensors to calculate the BB emissions in real time. Here, we present simulations of HRRR-Smoke for the August-September 2017 time period that is associated with one of the worst fire seasons in the northwestern US.

In this study we evaluate the HRRR-Smoke predictions of 3D distributions of smoke concentrations by using hourly PM2.5 measurements from the ground-based network and VIIRS satellite AOD data for this case study. The emissions of smoke near the surface and aloft (plume rise) and its transport on a regional scale in the model are analyzed in detail. We also evaluate the ability of the high-resolution model to capture the transport of smoke over complex terrain in the northwestern US.

Additional sensitivity simulations are conducted by enabling the smoke impact on radiation and microphysics in HRRR-Smoke. These sensitivity simulations allow us to estimate the impact of smoke on air temperature across the region, for example. We present an extensive verification of the HRRR-Smoke forecasts for meteorology by comparing the modeled temperature, moisture, cloudiness and precipitation over the CONUS domain for the case study. A new visibility parameterization, which accounts for smoke extinction, is used here to improve the visibility forecasts when high levels of smoke are present. In addition to the improvement of air quality and visibility forecasting, this study also helps to demonstrate the importance of the inclusion of aerosol within NWP models.

9AM.5

Characterizing the Climate Impacts of Brown Carbon over California. ANIKENDER KUMAR, Michael Kleeman, Christopher Cappa, Lynn Russell, *University of California, Davis*

Brown carbon (BrC) is an important component of the atmospheric radiation budget. Past studies analyzing the effects of BrC on climate change have been conducted at the global scale with limited ability to resolve regional details associated with targeted emissions control programs. These global studies have necessarily used simplified aerosol chemistry to represent the complex interactions between aerosols, clouds, and radiation. These features make it difficult for California to fully evaluate the climate effects of emissions control programs that seek to reduce ambient concentrations of BrC.

In this study we examine the effect of BrC absorption on regional scale over California. The source-oriented WRF/Chem (SOWC) model is used to track a six dimensional aerosol variable (X, Z, Y, Size bin, Source type, Species) through explicit simulations of atmospheric chemistry and physics. To the best of our knowledge, this is the first study to track BrC using source-oriented air quality model with external mixing. In source oriented external-mixture representations, particles of the same size can age to display different chemical compositions that depend on the chemical and hygroscopic properties of the primary seed particles initially emitted from different sources. A new mechanism is incorporated into this framework for formation of SOA from the reactions of phenol, glyoxal and methylglyoxal on aqueous aerosols in winter.

The SOWC model is applied for one year from Aug, 2014 to July, 2015 with 12 km resolution over California. Simulations are based on the regional emission inventory provided by the California Air Resources Board (CARB). Major BrC sources are identified as biomass burning, incomplete combustion of fossil fuels and secondary organic aerosols (SOA). The model results are compared with observed concentrations of biomass burning-organic aerosol (BBOA) and nitrate-related oxidized organic aerosols (NOOA) measured with an Aerodyne aerosol mass spectrometer (AMS) at Fresno, California. The direct effect of regionally emitted / formed BrC on radiative forcing at the top of the atmosphere is calculated. The influence of regional emissions control programs to reduce BrC and climate forcing are estimated.

9AM.6

Simulations for Estimating Dynamic Shape Factors of Aerosol Aggregates. Aniket Talele, Y.S. MAYYA, Jyoti Seth, *Indian Institute of Technology Bombay*

Aerosol aggregates are a common occurrence in nature and in various technological contexts, due to the ever-present process of coagulation. Soot particles formed in flames, metallic particles synthesized from vapor phase, particles produced by spray drying of suspensions are some of the well-known examples of aggregated particles. It is crucial to estimate the dynamical shape factors of the aggregates for describing their coagulational and depositional characteristics, in the atmospheric or in the respiratory tract. Unlike single particle systems, the dynamical behavior of aggregates is strongly governed by the interaction between the fluid and the individual constituent units and their spatial distribution. There have been several experimental and theoretical efforts in the past to describe the hydrodynamic behavior of aggregates (Sorensen, 2011). Semi-analytical approaches such as Kirkwood-Riseman approximation and simulation techniques such as Lattice-Boltzmann method or Stokesian Dynamics are some of the approaches used for evaluating their hydrodynamic resistances. Among these Stokesian Dynamics formalism is a comprehensive approach that incorporates fluid-particle and particle-particle interactions among the large number of primary particles. Particles interact via hydrodynamic forces transmitted through the solvent as well as short range inter-particle forces.

In these simulations, clusters of different fractal dimensions are constructed using Diffusion Limited (DLA), Reaction Limited (RLA) and Cluster-Cluster Aggregation (CCA) algorithms. A cluster of particles is represented as an assembly of spheres held together by either rigid bonds or soft Hookean springs. The latter aspect takes into account the change in shape of the aggregates subject to stress fields. Using the Stokesian Dynamics formalism (Brady and Bossis, 1988) configuration dependent hydrodynamic interactions are calculated, which account for the motion of particles relative to the fluid. Using Faxen's laws, far-field, many-body hydrodynamic forces are calculated by inverting a mobility matrix constructed from the first few terms of multipole expansions for two hydrodynamically interacting bodies. As this method is a good approximation only in the far field, close-range lubrication forces are calculated separately and accounted for in a pair-wise manner. Other non-hydrodynamic forces such as Brownian, colloidal, inter-particle, or external body forces can also be included.

In this talk, simulation estimates for the scaling exponent and pre-factors for drag forces experienced by rigid and deformable particle clusters will be presented. Apart from obtaining relationship between hydrodynamic radius and aggregate mass for different fractal dimensions, these simulations can also shed light on mechanisms of deformation of aggregates under various flow and settling regimes.

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9AM.7

Impact of the Assumptions of Soot Nanostructure and Aggregation on Particle Sizing Using Time-Resolved Laser-Induced Incandescence. MADHU SINGH, Randy Vander Wal, *The Pennsylvania State University*

Soot emissions contribute to deteriorating air-quality and have an adverse impact on human health and the environment. It has, thus, become imperative to characterize soot for its particle size, morphology, composition and optical properties, for instance, to better understand the material and the consequence of its formation. Towards particle sizing, time-resolved laser-induced incandescence (TiRe-LII) is one such non-intrusive, in-situ optical diagnostic technique used to estimate soot primary particle size. TiRe-LII uses the conductive cooling profile of laser-heated soot to infer primary particle diameter. Conductive cooling is believed to occur after approximately 100 ns of the laser pulse, with sublimation and radiation dominating cooling during the first 100 ns. Here, it is tested experimentally using three model carbon blacks with ranging particle diameters as measured by transmission electron microscopy (TEM). The carbon blacks are dispersed as an aerosol and irradiated by the primary harmonic, 1064 nm, of a Nd:YAG laser at a fluence of 200 mJ/cm^2. The incandescence signal, collected by a spectrograph-camera system, is temporally resolved by controlling and stepping out the gate delay in time, allowing the collection of detailed temperature-time profiles. Incandescence data is acquired as the particle cools, from which the particle's time-temperature history is extracted. Soot particle temperature is calculated by multi-wavelength pyrometry across a 600 nm spectral band by fitting the acquired incandescence spectra to Planck's black-body radiation law. Good fits to black-body profiles justify the use of a wavelength-independent emissivity with a value equal to unity. This assertion is supported by changed nanostructure and consequently, altered optical properties upon laser annealing. The effect of annealing on nanostructure is shown by TEM images. Aggregate morphology and primary particle size remain equivalent to the original material, while the particle's nanostructure changes. Based on Kirchoff's law, an alteration in optical emissivity post annealing is demonstrated by UV-VIS absorption, used here as a surrogate measure of the particle's emission. This data also shows a reduction in the material's optical band-gap after annealing, supporting increased π-conjugation and aromatic structure, all pointing to a changed and wavelength-independent emissivity. Primary particle diameters found from fitting experimentally measured TiRe-LII signals with existing analytical and numerical models do not match the particle diameters as directly visualized by TEM. TiRe-LII models typically assume point-contacting spheres and a constant accommodation coefficient in order to generate a temperature profile and infer particle size. The thermal accommodation coefficient is shown to be temperature dependent based on experimental conductive cooling profiles and differs substantially between these materials. Soot particles exist as aggregates and modeling them as point-contacting spheres is an over-simplification leading to inaccurate particle sizing. Aggregate structure in the form of intra-aggregate connectivity and shielding is an underlying cause for erroneous particle sizing. Effect of aggregation and the thermal accommodation coefficient as currently incorporated in current LII models is isolated and demonstrated individually, all other parameters being constant. Time-temperature profiles vary significantly as the degree of aggregation and value of the thermal accommodation coefficient change, pointing to inaccuracies in particle sizing by models.

9AM.8

How to Make Organic Molecules for New Particle Formation in Atmospheric Models: Recipes from the CERN CLOUD Experiment. HAMISH GORDON, Simone Schuchmann, Roy Lee III Mauldin, Matti Rissanen, Chao Yan, Lukas Fischer, Mario Simon, Martin Heinritzi, Ken Carslaw, CLOUD Collaboration, *University of Leeds*

New particle formation (NPF) in the atmosphere accounts for over half of global cloud condensation nuclei (CCN) in our simulations[1] with the GLOMAP model[2]. When organic molecules participate in NPF and in growth of nanometer-size particles, global CCN concentrations at the level of low clouds increase by around 20%.

The production of the low volatility, highly oxidised organic molecules (HOMs) that affect new particle formation in atmospheric models is usually fairly crude. New particle formation in regions dominated by organics is known to be affected by NOx, isoprene, and temperature, among other factors. The auto-oxidation process by which most HOMs are thought to form[3] is only starting to be understood (e.g. 4). Many models, including ours, do not account for the effects of different environmental and chemical conditions on this mechanism, and this leads to disagreement between the model and observations. For example, our model produces unrealistically high new particle formation rates in some regions, especially the Amazon[5].

In this study, we discuss ways to refine the treatment of HOM production in large-scale models, and thereby improve the agreement of our model of new particle formation and growth with observations. Yields of HOMs from the CERN CLOUD experiment arecombined with simplified reaction schemes derived from the Master Chemical Mechanism[6] to account for the influence of NOx and isoprene chemistry on HOM production. We implement a new HOM formation mechanism into the GLOMAP aerosol model and examine the effects on new particle formation and growth. The model is re-evaluated against measurement data and the implications for the indirect effects of aerosols on climate are discussed.

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9AP.1

Experimental Study of the In-Cloud Electroscavenging. ALEXIS DEPEE, Pascal Lemaitre, Anne Mathieu, Marie Monier, Andrea Flossmann, *French Radioprotection and Nuclear Safety Institute*

The scavenging of aerosol particles (AP) is of importance for understanding the atmospheric particles loading, which impacts both air quality and climate. In the case of a nuclear accident and the discharge of radioactive material, this understanding is a key to the forecast of radioactive dissemination and needed to protect populations. Far from the source, the AP scavenging is mainly due to the wet scavenging which combines two mechanisms: the AP removal by clouds (rainout) and the AP collection by raindrops (washout).

In most current models, the AP scavenging is often parameterized with empirical formulas issued from measurements including precipitation rates (Scott, 1982). No distinction is made regarding if scavenging occurred in the cloud or below in the precipitative region, while the microphysics effects which lead to the AP removal are significantly different. Indeed, there is no parameterization of the rainout whereas it has been shown both theoretically (Flossmann, 1998) and experimentally (Laguionie *et al.*, 2014) that rainout dominates the wet scavenging.

The lack of a detailed model for in-cloud AP scavenging can be explained by the difficulty to measure AP collection efficiencies by micron-sized cloud droplets; and even more to disentangle the different processes implied in the collection. For radioactive aerosol particles, the electrostatic forces are one of the factors which could significantly impact the AP collection by clouds since AP and cloud droplets are charged. Thus, few theoretical works using the theory of mirror charges introduced by Jackson (1975) have been undertaken. However, no experimental data is available in the literature to validate (or not) those models.

The present study attempts to fill this data gap through a novel experiment called IN-Cloud ElectroScavenging Chamber (INCESC) inspired by the Collision Ice Nucleation Chamber (CLINCH, Ladino *et al.*, 2011). The chamber mixes an online AP flow with a micron-size droplet jet to quantify the AP collection by droplets via a fluorescence analysis. A Differential Mobility Analyzer (DMA) is used to get a monodispersed AP size while the droplets are generated by a piezo-injector. A cooling system sets the chamber’s temperature to regulate the relative humidity. INCESC distinguishes itself from CLINCH by proposing a new system to control the charge of AP and droplets.

Finally, the measurements of the AP collection efficiencies by droplets for some AP and droplet charges and few AP radii are presented and compared to the theoretical model implemented for this purpose. These results reflect a next step towards the improvement of the AP scavenging model by strengthening the knowledge of the interaction between AP and clouds. A final stage will be to use these data to get a new parameterization of the in-cloud scavenging of heavily charged radioactive AP.

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9AP.2

Approximation to the Diffraction Limit of Three Dimensional Shapes Using the Scaling Approach. JUSTIN MAUGHAN, Christopher Sorensen, *Kansas State University*

A scaling approach for understanding features such as power laws and cross over points of the light scattered in the diffraction or m→1 limit, where m is the relative index of refraction is presented. The scaling approach is a semi-quantitative approach to describing the behavior of the structure factor of an arbitrary collection of scatterers, be it a dense three-dimensional particle, fractal aggregate or a collection of scatterers within a scattering volume. The focus here will be on single three-dimensional orientationally averaged homogenous particles. In the scaling approach, instead of considering the particle itself as being rotated, it is instead the scattering wave vector q that can take on all possible directions. Instead of being a vector q can be thought of as a spherical region with radius $q^{-1.}$ It will be shown that for three dimensional shapes such as hexagonal columns, spheroids, cylinders, and square columns the average behavior, power laws, and cross over points of the structure factor can be described by a single parameter ε which is the aspect ratio of the shape.

9AP.3

Characterization of Droplets Injected into Hyperbaric Atmospheres by the Flow Blurring® Mechanism. LUIS MODESTO-LÓPEZ, Alfonso Gañán-Calvo, *University of Seville*

In a general liquid atomization process a fraction of an energy input is transformed into surface energy. Particularly, in pneumatic atomization, the interaction of gas and liquid flows is typically accompanied by turbulent motions that lead to production of relatively small droplets.

An efficient liquid atomization method was developed by Gañán-Calvo (2005), known as Flow Blurring (FB). This method maximizes the surface area of the liquid flow at a minimum gas expense, thus resulting in a high atomization efficiency compared to conventional pneumatic techniques. The approach is also effective in preventing droplet coalescence. In a FB atomizer, an unexpected back-flow pattern in its interior, close to the atomizer outlet, produces small scale perturbations leading to an efficient mixing between the gas and liquid flows (see Gañán-Calvo, 2005; Modesto-López & Gañán-Calvo, 2018).

Typical FB atomizers are built with a simple yet robust design in which a liquid feeding tube is placed concentrically inside a gas feeding tube. The two fluids then interact in a zone nearby the outlet of the inner tube. Aerosol droplets, with a broad size distribution, leave the atomizer through a discharge orifice, spaced at a distance H from the tip of the liquid feeding tube. In these atomizers, the interaction of the liquid and gas flows is controlled by a geometrical parameter (ϕ), which is the ratio of H to the diameter (D) of the discharge orifice, as depicted in Gañán-Calvo (2005). FB atomizers find applications in many technological areas.

FB nozzles have been used in spectrometric techniques for generation of analyte droplets (Kovachev *et al.*, 2009) and in atomization of biofuels (Simmons and Agrawal 2012). Recently, we have proposed a direct atomization of water into a combustion engine with FB nozzles, aiming at reduction of emissions (Modesto-López and Ganán-Calvo 2017). The approaches that use water in combustion engines include either direct injection or mixing with the fuel (Sahin *et al.*, 2014). In both cases, the size of the droplets is a key parameter influencing the droplets' evaporation timescale and their transport characteristics, and thus combustion efficiency. Most of the research on these topics has been carried out at ambient or relatively low pressure conditions. However, FB in high-pressure environments, where many processes occur, remain largely unexplored. Thus, a detailed characterization of droplet size is of significant importance to understand in those environments.

In this work, we study the characteristics of sprays injected by FB nozzles into a chamber where a high pressure atmosphere is maintained. We coupled real-time visual methods with light scattering techniques to obtain the size distribution and the speed profile of aerosol droplets in the vicinity of the FB nozzle. The key process parameters controlling FB atomization are the liquid flow rate, Q, the inlet gas pressure, Po, the chamber pressure, Pi, and thus the pressure difference, ΔP = Po - Pi. We also investigated a wide range of ΔP values for three different liquid flow rates to obtain a correlation in terms of dimensionless parameters.

The approach presented in this study may be a guideline for implementation of FB in high-pressure applications, for instance, in combustion technology.

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9AP.4

Capillary Oscillations in the Transient Mode of Flow Focusing: Comparison Between Experimental Measurements and Numerical Results. VICTORIEN MAMET, Michel Matton, Stéphane Gasser, Patrick Namy, Jean-Marc Dedulle, *LMGP - Grenoble INP / UGA, DBV Technologies*

Among droplet generation technologies, the flow focusing technique is a major process due to its control, stability, reproducibility and adaptability to the biomaterial handling. The principle is to create a spray from the coflowing of two fluids. In the transient flow, there is a oscillation of the liquid motion which has proved to be periodic. It has first been studied in the 1990s experimentally [1], and new phenomena inherent to the physical dynamics of the fluid flows have been found by numerical modeling.

We perform a series of experiments to study the transient mode in flow focusing, more particularly the behavior of the period of oscillation $\tau=T/T_0$ versus the Reynolds number Re_l. We then compare it to the results of numerical simulations, performed on a model developed in [2] in order to give more range to our results.

The experiments are conducted with a custom made flow focusing device and measurement tools adapted for the range of the observations wanted.

The experiments show that during one period the liquid flow is subjected to several micro-oscillations called capillary oscillation during the oscillation, as predicted in numerical simulations. We find a step-like decreasing behavior for the dimensionless period versus the liquid Reynolds number. The behavior of the capillary oscillation number depending on this Reynolds number is in excellent correlation with the numerical results.

These results highlight the discontinuous response of the fluid flow depending on slight variations of the physical parameters and may allow to give some indicator of the flow regime.

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9AP.5

"Particle Formation" vs. "Particle Growth": Robust Metric for Determining the Onset of Condensational Growth of Nanoparticles.

TINJA OLENIUS, Dominik Stolzenburg, Lukas Pichelstorfer, Paul M. Winkler, Kari Lehtinen, Ilona Riipinen, *Stockholm University*

Understanding the mechanisms of nanoparticle formation and growth from vapors is essential for resolving nucleation and condensation phenomena. Correct representation of these processes in atmospheric models is also a prerequisite for quantifying atmospheric aerosol particle loadings: Gas-to-particle conversion is assessed to make a substantial contribution to the total aerosol number, but these estimates are highly sensitive to assumptions on the growth dynamics of the smallest nanoparticles below ca. 5-10 nm in diameter. For large enough particles, the vapor-particle mass exchange driving particle growth or evaporation can be described assuming a continuous flux of vapor onto the particle surface. However, this description does not apply to the smallest nanoparticles. Instead, at the smallest end of the particle size spectrum, particle formation and growth involve stochastic fluctuations in particle size due to discrete molecular collision and decay processes. The size regime where the discrete effects become negligible, indicating the onset of condensation-driven growth, has not been addressed to date.

In this work, we derive a simple and robust metric for quantifying the size regime where stochastic effects cannot be omitted for arbitrary molecular systems, based on theoretical considerations on the particle size distribution function. The proposed metric is confirmed by application on synthetic data, generated by molecular-resolution simulations of sub-10 nm particle populations representative of atmospheric nanoparticles, as well as on laboratory observations of particle formation. The results show that the significance of stochastics can be reliably assessed based on the shape of a measured nanoparticle size distribution, with no need for knowledge of the properties of the nucleating and condensing vapors.

The results raise important points regarding the interpretation and utilization of observation data. For atmospheric nanoparticle formation, the size regime at which condensation flux modeling becomes inapplicable is estimated to be below sizes of typically a few nanometers, depending on the exact chemical system in question. At these very small sizes, interpretation of experimental observations relying on condensation modeling may lead to erroneous conclusions on (1) the properties of the condensing vapors when fitting a condensation model to experimental data, (2) "missing" condensing species when observations cannot be reproduced by the model, and (3) the thermodynamics of nanoparticle growth, including the presence and magnitude of Kelvin barriers, when the observed time evolution of the particle size distribution is used to deduce condensational growth rates. To avoid such misinterpretations and to reliably extract information on particle formation mechanisms from experiments, constraining the limits of condensation modeling is necessary. The approach presented in this work provides a means to quantify these limits with a reasonable accuracy, building on the development of robust and generalizable data analysis tools.

9AP.6

Characterizing the Homogeneous Nucleation of Carbon Dioxide in a Supersonic Laval Nozzle. KAYANE DINGILIAN, Yensil Park, Barbara Wyslouzil, *The Ohio State University*

Understanding and characterizing the nucleation of carbon dioxide (CO_2) has significant implications on technologies used to assessing and countering climate change. CO_2 nucleation is also relevant on planets and other extra-terrestrial bodies where CO_2 dominates the atmospheric and cloud compositions. We studied the homogeneous nucleation of carbon dioxide in the carrier gas argon for varying concentrations of CO_2 up to approximately 40 mole percent in a supersonic nozzle. Using position resolved pressure trace measurements (PTM), we determined the pressure, temperature, and characteristic time corresponding to the phase transition. In our nozzle, we reached temperatures as low as 62K and pressures as low as 1200 Pa. We found the onset of nucleation of carbon dioxide took place between 83 and 93K with partial pressures of CO_2 ranging from 84 to 784 Pa. The position of onset initially moved upstream then shifted back downstream with increasing mole fraction of CO_2. This behavior indicated competition between the saturation of CO_2 with increased material and the thermodynamic properties of the CO_2-argon mixture. The characteristic nucleation time ranged from 10 to 26 microseconds and mirrored the trend seen in the position of onset. Small angle x-ray scattering (SAXS) measurements will be used to determine the aerosol number density and thus the experimental nucleation rate. The onset data collected in these experiments were located in the solid region of CO_2's phase diagram but we will use SAXS together with Fourier transform infrared spectroscopy (FTIR) measurements to try to discover which phase of CO_2 condenses first. Experimental results will be compared to classical nucleation theory and other models to help mend the gaps between predictive methods and reality.

9AP.7

Heterogeneous Nucleation onto Monoatomic Ions and the Role of Stable Pre-nucleation Clusters. Christian Tauber, Paul E. Wagner, Paul M. Winkler, Christopher Hogan Jr., ANNE MAISSER, *University of Vienna*

The investigation of the fundamental processes that enable and predict phase change is of great interest. Both homogeneous and heterogeneous nucleation/condensation processes are applied for e.g. nanoparticle synthesis, but also are responsible for new particle formation (NPF) in the atmosphere.

With advances in aerosol instrumentation towards observation of smaller and smaller particles an increasing attention was drawn to the investigation of the process of heterogeneous nucleation for seed particles with diameters down to the Kelvin diameter, and even below. A universal theory predicting heterogeneous nucleation, especially for particles smaller than the Kelvin diameter, is still missing, and development is limited due to the lack of meaningful experimental measurements. Accurate, well-defined measurements of activation probabilities require highly monodisperse nuclei and uniform supersaturations (Fernandez de la Mora (2011). Aerosol Science and Technology. 45(4):543-554). This still is difficult to achieve using general state-of-the-art aerosol instruments.

In this study we were able to overcome these experimental challenges by using highly specialized aerosol instruments that can meet both conditions: on the one hand a high resolution and transmission DMA for the size selection of highly monodisperse seed ions of defined chemical composition, and on the other hand an expansion type CPC for exposing the seed ions to a well-defined uniform supersaturation. In addition to the experimental work, we compared the results to existing theories by applying the classical nucleation theory (CNT) for the case of insoluble and perfectly wetting seed particles.

We examined the nucleation probability of monoatomic ions upon introduction of n-butanol into the size analyzing nuclei counter (SANC) (Wagner et al. (2003). Phys. Rev. E67:021605-1). With it, we could directly measure the onset saturation ratio and the additional number of n-butanol molecules to build a critical cluster by applying the Gumbel distribution. Furthermore, by applying a vapor uptake model we were able to calculate the mobility equivalent diameter of the ions at partial pressures of n-butanol below saturation (A. Maiβer & C. J. Hogan (2017) ChemPhysChem. 18(21):3039-3046). With these results and the assumption that the seed ions are spherical and perfectly wettable, we were able to calculate the critical cluster size for different monoatomic ions of both polarities. In total, we were able to quantitatively characterize the heterogeneous nucleation process for the pre-nucleation and critical nanoclusters using monoatomic singly charged ions of both polarities as seeds. In view of the small cluster sizes the prediction by the Kelvin-Thomson model can still be considered as reasonably accurate.

9AP.8

Original Approach for Determining Surface Binding Energy of Particle-adsorbed PAHs Using L2MS Signal Decay. MARIN VOJKOVIC, Dumitru Duca, Yvain Carpentier, Michael Ziskind, Alessandro Faccinetto, Cristian Focsa, *Université de Lille*

We present an original method for determining surface binding energy of Polycyclic Aromatic Hydrocarbons (PAHs) on black carbon, using signal decay in our Two-Step Laser Mass Spectrometer (L2MS). The reactivity and toxicity of soot particles is driven by the processes on their surface, where the nature and the strength of chemical bonds play an important role. Therefore, the research into the basic chemical properties of PAHs and their interactions with carbonaceous particles can yield valuable insights into soot chemistry, formation and health effects.

The L2MS technique used in our laboratory allows probing the surface chemical composition with great precision (Faccinetto et al. 2015). The two-step desorption-ionization method gives us high sensitivity in sample analysis. In addition to studying real soot, we use laboratory-made samples, synthesized by adsorbing well-determined amounts of selected PAHs onto black carbon particles to reach sub-monolayer coverage. This artificial soot allows us to study the PAH surface chemistry in controlled conditions.

The new approach for surface binding energy determination consists in measuring the shot-by-shot signal decay in L2MS. The method is derived from the measured total number of molecules desorbed after a given number of laser shots (Zhigilei et al. 1999), based upon the assumption of dominantly thermal desorption at low laser fluences (Dreisewerd et al. 1995) Two approaches are used for the binding energy measurement. For the first one, the signal intensity of the peak corresponding to the PAH of interest is recorded for each laser shot. The data is fitted with the pseudo exponential decay of number of molecules in n laser shots. From there, the unknown parameters are then retrieved. For the other approach, the mass spectrum is recorded by averaging the signal over 50-100 laser shots. In this approach, the sample is moved after each laser shot, ensuring that new area of surface is irradiated each time. Therefore, the intensity measured corresponds to the average intensity of the first laser shot. By recording the spectra in this manner, we are able once again to extract the binding energy of the adsorbed species. The two different approaches complement each other helping to achieve a more precise result by reducing the uncertainties introduced by fluctuations in laser fluence or possible non-homogeneous distribution of the molecules on the sample surface.

These results are presented as proof of concept for the new method, which, with refinement and higher precision in measurements, could enable us to identify different types of surface-molecule bonds.

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9BA.1

Bioaerosol Transmission: Experimental Replication of Natural Processes. RICHARD THOMAS, *Dstl*

Aerosol generation, transport and inhalation in natural environments will be reviewed to provide context for experimental replication of these processes for understanding disease transmission, epidemiological risk analysis and development of therapeutics. New data and evidence from the literature is presented to highlight the complexity of interpretation and extrapolation of data concerning natural and experimental bioaerosols.

9BA.2

BioAerosol Generation Methods. JAY D. EVERSOLE, Cathy S. Scotto, *Naval Research Laboratory*

This presentation will review recent methods of bioaerosol generation and assess their advantages and disadvantages. The term bioaerosol is taken here to be aerosol particles that includes, but is not restricted to microorganisms, so that particles composed of any biogenic or biomolecular material would be included. Unfortunately, this is such a broad category, in which each organism or specific material has a multitude of somewhat unique specific characteristics that it is difficult to organize along general principles. Rather than simply attempt to summarize and catalog recent literature on bio-aerosol generation results, we approach this question in terms of available methods. In broad stroke, bioaerosol generation for experimental purposes falls into one of two methods: (a) producing droplets of liquid suspension, or (b) directly producing dry particles from powdered sample material. For both these approaches a number of specific devices or methods exist, each of which will affect the resulting aerosol in terms of its composition, aerodynamic diameter (D_{ae}), and relevant biological function(s).

As with all aerosols, particle composition and D_{ae} distribution are important aspects to either control or characterize, but bioaerosols have a large range of additional factors that characterize their biological state. Examples of biological characteristics include: enzymatic activity, toxicity, culturability, viability, and infectivity. Specific factors will depend on both the biological material being addressed as well as the purpose, or application, of the aerosol experiments. For most of the work referenced in this review, the materials considered are microorganisms and either viability or culturability are critical parameters for the resultant aerosol.

Far from a simply pedantic concern, the preparation and characterization of a bioaerosol material can have direct and significant consequences for the data analysis and interpretation of experimental measurements. Biodegradation can and generally does occur on a continuous basis even during sample storage, and the process of aerosolizing the sample will have its own degradation effect. Once the particles are airborne, then experimentally one has to account for mechanical loss of particles to surfaces and gravitational settling, which is referred to as aerosol decay, but additionally there will be bio-degradation effects due to the new physical condition of being a particle suspension in air, which generally will be greater than the decay rate as a bulk sample. Since these effects are measured in terms of populations of particles/organisms, it is important to characterize and engineer sample homogeneity. To illustrate, suppose one wants to determine the effect of an environmental parameter on viability of a specific organism as a bioaerosol. To establish a baseline, or control, consider that the rate of degradation may also depend on sample growth protocol, growth stage at harvesting, method of preparation for being aerosolized as well as aerosol generation method itself. In other words, the measured result is to some extent a package which includes the detailed sample history. Additionally, it is extremely rare for an organism to be aerosolized by itself, and to the extent that the organism is just one constituent in the presence of other material(s) adds more variable(s) that potentially can modify results.

This brief description should provide some appreciation for the extensive list of characteristics, initial conditions and experimental variables that can arise when attempting to quantify biological materials as aerosols. In light of this situation, one could argue the necessity of establishing some sorts of standards through which results from different experiments could be compared. We will illustrate our perspective using current popular methods and discuss the positive and negative features of each.

9BA.3

Understanding the Principles of Bioaerosol Sampling. GEDIMINAS MAINELIS, *Rutgers, The State University of New Jersey*

Bioaerosols include airborne viruses, bacteria, fungi, pollen and their products; the size of bioaerosol particles can range from nanoscale to micron size. Various application of bioaerosol research, from exposure assessment to the investigation of bioaerosol role in atmospheric processes, require reliable bioaerosol sampling and detection methods. While the same physical principles that are applied to collect non-biological aerosol particles can also be used to collect bioaerosols, bioaerosols present an additional challenge; their viability, morphology, cell integrity, DNA structure, etc., have to be maintained to enable reliable bioaerosol analysis and identification. Thus, when sampling is performed to identify and quantify airborne biological particles, not only sampling efficiency but also collection mechanism, sample volume, sampling duration, concentration rate and accuracy of detection are important parameters.

This presentation will review traditional and emerging techniques for bioaerosol sampling and will discuss factors affecting the accuracy of bioaerosol sampling and determination, including collection efficiency of the collectors, sample volume and sampling duration, and concentration rate. Special focus will be paid to sampling techniques and parameters that allow minimizing potential damage to microorganisms during their collection. Analytical bioaerosol techniques and protocols that allow evaluating the performance of bioaerosol collectors will also be discussed.

9BA.4

Laboratory Systems for Biological Aerosol Experimentation and Testing. JOSHUA SANTARPIA, Shanna Ratnesar-Shumate, *Sandia National Laboratories*

Laboratory aerosol studies require careful control and measurement of the aerosol in addition the test environment. Biological aerosol studies can be even more complex, and studies that explain the potential changes to biological aerosol due to environmental factors are only beginning to emerge. In the last several years, many studies have used field and laboratory measurements to begin to understand the factors that may affect biological aerosols and their measurement. These factors include chemical and physical changes to the biological aerosols as well as and changes in the environment both of which may impact sensor performance and the accuracy of detection, identification or quantification the biological aerosols. If not properly controlled and quantified, environmental factors may unknowingly lead to uncertainty and variability in experiments and poor performance of measurement techniques. This talk will review laboratory test systems utilized in biological aerosol studies and factors that may impact biological aerosol measurement in both laboratory and field experiments. Laboratory systems to control for environmental impacts as well as the potential effect of the test systems on measurements, such as physical losses during aging studies, or variations in temperature, solar spectrum, and relative vs. absolute humidity effects will be discussed. A better understanding of how to design, optimize, and characterize bioaerosol test systems will ultimately improve our understanding of aerobiology and help to improve biological aerosol measurement studies and meaningfulness of the data.

9BA.5

Bioaerosol Sampling in Field surveys. TIINA REPONEN, *University of Cincinnati*

The choice of a bioaerosol sampling method depends on the purpose of the sampling: is sampling conducted for verification of the presence of microbial problems, identification of the source, monitoring the efficiency of control methods or assessment of the human exposure. When choosing a sampling method, one also has to consider which analysis method would give most relevant measures for the question asked. This, in turn, may limit the choice of sampling methods available. A wide variety of sampling methods are available for assessing microorganisms in indoor environments. These can be categorized into four main groups: air sampling, dust sampling, surface sampling and building material sampling. This presentation will review the traditional and modern sampling techniques available with a focus on air sampling and will discuss the advantages and disadvantages of the choices available.

Air samplers are based on well established aerosol collection mechanisms, such as impaction, interception, diffusion, electrostatic attraction, and gravitational settling. The same physical principles that are applied to non-biological particles can be applied to bioaerosol sampling in terms of sampling efficiency of a given particle size range. An additional consideration for sampling microorganisms is the ability to maintain the biological property that is used in the analysis, e.g., culturability of cells or integrity of genetic material. Also, particle bounce can be a pronounced problem in impaction sampling of spores. Although air sampling should be the most representative of respiratory exposure, traditional air sampling methods have several limitations. Most methods cannot be used for assessing long-term exposure to bioaerosols. The sampling period of most commonly used commercially available instruments (e.g., Burkard, Andersen, Air-O-Cell) is limited to 5-20 min while the bioaerosol concentrations have wide temporal variation, particularly if an active source is present, such as in mold-problem homes. Therefore, short-term sampling often fails to detect certain species, which are present in low concentration but may be important for the subsequent health effects. Several new samplers have recently been developed specifically for the collection of bioaerosol particles, e.g., Viable Virus Aerosol Sampler (VIVAS) and Rutgers Electrostatic Passive Sampler (REPS). There are also a few direct-reading instruments, most of which are based on laser-induced autofluorescence of biological material, but these have limitations in identifying the specific microbial types.

For building investigations, direct source evaluation techniques (bulk, surface, and dust sampling) may be preferred as these allow the investigators to collect extensive information about the source. The disadvantages of dust sampling, especially from the floor, are that the sample may not adequately reflect human inhalation exposure and that the age of floor dust is often not known. An alternative is a long-term collection of settled dust by placing dust sampling platforms at a certain height in the indoor environment. Another approach is to use a specially-designed aerosolization chamber that releases biological particles from contaminated surfaces by air currents and vibration (e.g., Fungal Spore Source Strength Tester, FSSST, and Particle-Field and Laboratory Emission Cell, P-FLEC). This approach can give the worst-case scenario for the possible airborne concentration of biological particles that can be released or resuspended from the surface under investigation.

As each technique has unique advantages and disadvantages, it is often beneficial to use multiple techniques in each investigation. Also, it should be kept in mind that results between different studies could be compared only if same sampling and analysis methods were used.

9BA.6

Factors Influencing Interpretation of Laser-Induced Fluorescence (LIF) Instruments for Bioaerosol Measurement. J. ALEX HUFFMAN, *University of Denver, CO*

Several classes of real-time characterization techniques have been developed and applied recently for the analysis of bioaerosols, with increasing attention in the last decade. Single-particle spectroscopy based on ultraviolet laser-induced fluorescence (UV-LIF) is currently among the most widely used technique for real-time detection and characterization of bioaerosols. The principle of utilizing fluorescence spectroscopy to detect and characterize bioaerosol hinges on the idea that most biological material contains a reasonably small set of characteristic fluorophore classes, e.g. aromatic amino acids or riboflavin, that can be used to differentiate it from non-biological material. Most online UV-LIF techniques for bioaerosols detection thus require components of the aerosol to exhibit intrinsic fluorescence, or autofluorescence. Many instruments have been developed by universities, government labs, and military research organizations. Built on their decades of work and to capitalize on the ability to detect and characterize bioaerosol properties in (semi)-real time, a host of companies have begun offering UV-LIF bioaerosol sensors over the last 10-15 years. Instruments such as the UV-APS (TSI) and WIBS (Droplet Measurement Technologies) have been widely utilized and employed in countless scientific studies, and instruments such as the Bioscout (Environics), Rapid-E (Plair), SIBS (DMT), IMD (BioVigilant), and MBS (Univ. Hertfordshire) are just a few of the many other UV-LIF instruments now available on the commercial marketplace.

High quality interpretation of biological aerosol measurements using fluorescence techniques must also necessarily include an understanding of the limitations of using fluorescence to measure these particles. For example, fluorescence intensity increases strongly as a function of particle size and is especially dependent on surface properties of the particle (e.g. membrane opacity). Detector sensitivity also usually varies as a function of wavelength. As a result, particle detection can be heavily influenced by technical details that influence whether a given particle will be above the noise threshold and thus be categorized as fluorescent or not in a given spectroscopic channel. Different instrument types and different operators may employ very different thresholding strategies, which can dramatically influence the interpretation of results. As a result of these factors, results from different instrument types are often challenging to compare and it is critical that end users properly keep these factors in mind when drawing conclusions from fluorescence-based bioaerosol spectrometers.

Significant work over several decades supported the development of the general technologies, but efforts to systematically characterize the operation of new commercial sensors has also remained somewhat lacking. Specifically, there have been gaps in the understanding of how different classes of biological and non-biological particles can influence the detection ability of LIF instrumentation. A solid understanding of interfering species, which may be very different if e.g. the instrument is operated in a remote field location or inside an occupied building, is critical. Factors related to aerosolization in laboratory studies can also significantly influence fluorescence properties of aerosol. For example, growth conditions of microorganisms may influence their viability state as well as other physical properties, and the choice of growth media can frequently introduce false-positives for fluorescence detection. Lastly, increasingly complex data analysis methods have been applied to commercial UV-LIF sensors, ranging from relatively simple, binary categorization of fluorescent vs non-fluorescent, to more complex applications of clustering or machine-learning algorithms. It is important to understand potential pitfalls of a given analysis style to optimize data interpretation, but this is often not a trivial task and can require significant laboratory study.

For this presentation I will give a brief overview of some of the laboratory, instrumental, and analysis factors involved in optimizing the quality of results for UV-LIF methods for bioaerosol sensing.

9BA.7

Aerosol Dosimetry and Extrapolation between Species. MICHAEL OLDHAM, *Altria Client Services LLC*

Aerosol dosimetry is a critical link between exposure to inhaled particulate matter and potential toxicity. Aerosol dosimetry can also be used as a tool for extrapolation of results between species for inhaled material. Viable aerosols can present unique aerosol dosimetry challenges/opportunities when used in in-vitro and in-vivo studies. Similar aerosol dosimetry challenges/opportunities exist when extrapolation between species is done for viable aerosols.

The goals of in vitro dosimetry studies have evolved from simply knowing the exposure concentration in the culture, to determining the cell exposure concentrations, as well as the cell surface dose that causes the response. Now, the goal is to determine the internal cell dose that results in the response, and even to determine the dose at the receptor inside the cell. Recent use of 3D human tissue constructs combined with air-liquid-interface (ALI) in-vitro exposure systems has enabled direct aerosol exposure similar to what occurs in the respiratory system. Coupling the 3D human tissue constructs, ALI exposure methods, aerosol dosimetry measurements with 21st century “omic” techniques are providing new insight to disease processes.

Well defined aerosol dosimetry (spatial and temporal) is essential to obtain the most insight from in-vivo studies regardless of the exposure method (whole body, nose-only, individual mask, nasal cannula, etc.). Aerosol dosimetry for in-vivo studies has evolved from measuring exposure concentration to measuring biomarkers of exposure and/or biomarkers of potential harm and correlating those measurements with predictions of doses delivered to specific locations within the respiratory tract. Combining measurements of biomarkers of exposure and/or potential harm with location specific tissue dose predictions has shown in some cases that dose rate is more important than the total delivered dose.

Use of aerosol dosimetry for species extrapolation is complicated by some of the inherent species differences and by the lack of specific information regarding those potential differences. Important species differences include particulate inhalability, respiratory tract anatomy, physiology, and the anatomical variability of the respiratory tract anatomy. For example, recent use of aerosol dosimetry in two types of mice demonstrated that respiratory tissue sensitivity to inhaled methacholine is 50% of previously measured values.

Aerosol dosimetry for viable aerosols is a multi-factorial process that not only requires knowledge of the physical/chemical aerosol properties and their potency, but also the physical/chemical properties of the exposure environments (in-vitro setup, in-vivo setup, species specific respiratory tract anatomy and physiology). Continued development of and consistent use of appropriate aerosol dosimetry techniques can facilitate better extrapolation of in-vitro to in-vivo results and extrapolation between species for inhaled material.

9BA.8

Conducting Inhalation Exposures Using Bioaerosols; Infectious Microorganisms and Toxins: Concepts and Lessons Learned. ROY BARNEWALL, *Battelle, Columbus Ohio*

Medical countermeasures such as vaccines and pharmaceuticals that are used to protect against or treat diseases caused by biological agents (bacteria, viruses and toxins), are often evaluated for efficacy against these agents via inhalation, which is a probable route of exposure from a natural infection, accidental release or deliberate release. Testing of animal models of infection or disease need to be conducted safely by using well characterized biological material and well characterized inhalation systems with highly controlled procedures and processes in order to ensure reproducibility and consistency in the inhaled or presented dose of the microorganism or toxins. This is especially true for research which will be used in support of product licensure by the U.S. Food and Drug Administration.

This presentation will briefly outline the universal components of an inhalation exposure system and a few of the various types of exposure systems available and what is used by Battelle. Additionally, the practical and safety aspects of performing inhalation dosing using these agents will be discussed. The primary focus of the presentation will be on the concepts of performing bioaerosol exposures and physical properties of the environment that can affect the agent and the agents themselves and how they may impact the bioaerosol. The presentation will conclude with lessons learned over the years of performing bioaerosol testing. The effects of agent preparation, sampler choice, temperature and relative humidity, volume within the sampler, and agent strain differences on how they may affect the characterization of an aerosol system were evaluated. Some examples that will be discussed are that testing revealed that the optimal sampler chosen for dose quantification is primarily dictated by the biological agent being tested. For many bacterial aerosols an impinger was the most practical while gelatin filters were optimal for some viruses. The choice of media used and how the agent is prepared will have an effect on viability as will the temperature and humidity levels. The effect of temperature and humidity varied based on the agent with high temperature and humidity (70% and higher) predominately resulting in lower viability or infectivity compared to higher viability or infectivity at lower relative humidity (approximately 50%). Once these different factors are optimized and controlled, will minimize intra-day and inter-day variability and allow for the reproducible dose results within a study and between studies.

9CA.1

Aerosol Optical Properties and Climate Implications of Emissions from Traditional and Improved Cookstoves.

GEORGES SALIBA, R. Subramanian, Kelsey Bilsback, Christian L'Orange, John Volckens, Michael Johnson, Allen Robinson, *Carnegie Mellon University*

Cookstoves are a substantial global source of black carbon (BC) and brown carbon (BrC) particles which are climate-warming agents. Additionally, exposure to particulate matter (PM) from solid-fuel cookstoves is responsible for more than 4 million premature deaths worldwide, according to the World Health Organization. To reduce health, climate, and other environmental impacts, decades of research has gone into developing “improved” which aim to reduce emissions and/or exposure; however, measurements of real-cooking events indicate that improved cookstoves emit a higher BC fractions in emission compared to traditional cookstoves. Furthermore, the potential climate implications of a large-scale deployment of improved cookstoves remain uncertain due to limited (and variable) published field data of optical properties from cookstove emissions.

We used state-of-the-art instrumentation to measure aerosol optical properties from fresh emissions from 18 different cookstove/fuel combinations; the cookstoves tested include wood-burning three-stone fires, natural draft rocket cookstoves, charcoal cookstoves, and forced-draft cookstoves. The cookstoves were tested in the laboratory using the Firepower Sweep Test to characterize emissions across a wide range of cookstove power outputs. We used our large dataset to investigate differences in optical properties with varying cookstove technology, fuel (wood versus charcoal), and operation conditions. The BC/PM metric explained the measured variability in optical properties (R^2=0.9) and performed significantly better than other operational metrics, such as modified combustion efficiency (R^2=0.3) and firepower (R^2=0.1). We developed semi-empirical parametrizations (consistent with Mie theory) of the mass absorption cross-section per BC mass (MAC_{BC}), absorption angstrom exponent (AAE), and single scattering albedo (SSA) as a function of BC/PM. We measured increase in MAC_{BC} (from 10 m^2/g to 40 m^2/g), SSA (from 0.2 to 0.9), and AAE (from 1 to 5) with decreasing BC/PM, independent of cookstove technology. These measurements suggest that with decreasing BC/PM there is increased coating around BC particles and increased contribution from BrC to absorption. these findings are consistent with BC-mixing state from single-particle soot photometer (SP2). Finally, we found little dependence of the measured intensive optical properties on cookstove technology or fuel.

A key outcome from our analysis is that the measured increase in MAC_{BC} with decreasing BC/PM was inconsistent with current model treatments of the optical properties of cookstove emissions. Models assume internal mixture of BC and non-BC material and BrC absorption based on biomass burning parametrizations; however, our data indicate that this approach may not reflect real-world emissions. We compared measured MAC_{BC} with Mie theory predictions for different particle mixing-states and with and without BrC and found that treating BC and non-BC materials as internally mixed overestimates the measured MAC_{BC}. Our new parametrizations include contributions from lensing, mixing-state, and BrC to absorption and can be used in emission inventories, which contain BC/PM data. Furthermore, our data indicate that: (1) intensive optical properties measured in the laboratory using the Firepower Sweep Test are representative of field measurements, and (2) for relevant cookstove operation, the enhancement in MAC_{BC} is dominated by mixing-state and lensing and not BrC.

Finally, we combined our parametrizations of intensive optical properties with field emissions data from the literature to estimate the direct radiative effect of emissions for different cookstove technologies, using a simple forcing efficiency metric. We predict only 20% climate benefits from improved cookstoves compared to traditional ones (differences not statistically significant), but more than 50% reductions in PM mass emissions (statistically significant differences). We predict that the large-scale deployment of improved cookstoves will likely result in a modest reduction in the direct radiative effect from emissions.

9CA.2

Light Absorption by Carbonaceous Aerosol Emissions from Biomass Cookstoves in India. APOORVA PANDEY, Sameer Patel, Pratim Biswas, Shamsh Pervez, Rajan K. Chakrabarty, *Washington University in St Louis*

Combustion of solid biomass in traditional cookstoves in south Asia is the largest source of carbonaceous aerosols emissions in the region. Estimates of the radiative impact of aerosol emissions from biomass cookstoves have a high level of uncertainty arising from the underlying uncertainties in aerosol mass concentration distributions and optical properties–key input parameters in climate models. As a step towards resolving the uncertainties, our objectives were to (1) develop particulate mass emission factors for in-field operation of traditional biomass cookstoves, and (2) estimate wavelength dependent Mass Absorption Cross-sections (MAC) of the emitted aerosols and their light absorbing organic carbon (LAOC) components.

A field study was conducted in Raipur, Chhattisgarh (a central Indian state) in December 2015. Common types of biomass fuels from different regions of India were used in a traditional mud chulha to prepare typical meals in a household kitchen. Particle samples were collected on Teflon and quartz fiber filters during the ignition, steady flaming and smoldering phases of the combustion cycle. The Teflon filters were used for gravimetric analysis and UV-vis spectrophotometry. Thermo-optical (IMPROVE-TOR) analysis on the quartz filters yielded the elemental and organic carbon fractions. Emission factors (PM2.5, EC, OC and CO) were calculated using the carbon balance method. These emission factors together with the thermal fractions of the total carbon content of different fuels were compared with existing lab-based profiles. Empirical relationships between filter transmission spectra and particle light absorption were developed through laboratory studies of biomass burning. These relationships were applied to the spectrophotometer data to calculate the total aerosol MAC, which was apportioned to Black Carbon and LAOC using the two-component model. The total contribution of LAOC to aerosol light absorption was estimated by integrating its absorption coefficient with solar irradiance in the 300-900 nm wavelength range. The links between carbonaceous aerosol composition (OC-to-EC mass ratios and thermal carbon fractions) and aerosol optical properties are explored.

9CA.3

Estimation of Brown Carbon in PM2.5 Samples from Long-term Networks. XIAOLIANG WANG, Judith Chow, Brandon Daub, Steven Gronstal, L.W. Antony Chen, Mark Green, John Watson, *Desert Research Institute*

Black carbon (BC) and brown carbon (BrC) aerosols are light-absorbing substances that affect the Earth's radiative balance. While BC absorbs light across the visible spectrum, BrC primarily absorbs light at wavelengths less than 500 nm. The emission sources and climate effects of BC are widely studied and relatively well understood. In contrast, despite increasing interest in BrC aerosols, there is a large degree of uncertainty about their abundance, source attribution, and environmental/climate impacts, partially owing to a lack of BrC quantification at many different times and locations. Since 2016, BrC is being measured in U.S. chemical speciation networks using a thermal/optical carbon analyzer with seven wavelengths ranging from 405 to 980 nm. Outputs include estimates of aerosol absorption and charring corrections at each wavelength. A power-law fit through the light attenuation spectra yields the Absorption Ångström Exponent (AAE). BrC light absorption is estimated by subtracting the BC contribution with an AAE of 1 for each of the shorter wavelengths. This study evaluates the multiwavelength thermal/optical carbon measurements from the U.S. Interagency Monitoring of PROtected Visual Environments (IMPROVE) and Chemical Speciation Network (CSN) (~300 sites) for 2016 (~30,000 samples) to better understand the abundance and temporal variation of carbonaceous aerosols in the U.S. It is shown that the analyses maintain continuity with the long-term OC and EC databases for these networks. On average, non-urban IMPROVE samples show higher fractional BrC absorption than urban CSN samples, owing to greater influence from biomass burning and aged aerosols, as well as to higher primary BC contributions from engine exhaust at urban sites. The AAEs are higher at the IMPROVE than at the CSN sites. Sequential samples taken during an Everglades National Park wildfire illustrate the evolution from flaming to smoldering, with the BrC fraction increasing as smoldering begins to dominate the fire event. Characterization of light absorption properties of laboratory-generated BrC surrogate compounds demonstrate the feasibility of using the surrogate compounds' mass absorption efficiency to convert BrC light attenuation to BrC mass contributions to the carbonaceous fraction of $PM_{2.5}$.

9CA.4

Pinning Down the Highly Variable Light-absorption Properties of Brown Carbon. RAWAD SALEH, Zezhen Cheng, Khairallah Atwi, *University of Georgia*

Combustion of biomass fuels contributes a significant portion of atmospheric brown carbon (BrC), the light-absorbing fraction of organic aerosols. BrC exhibits highly variable light-absorption properties, with imaginary part of the refractive indices (k) reported in the literature varying over two orders of magnitude. There is a major gap in the understanding of this variability, posing a challenge to accurately representing brown carbon in radiative-transfer calculations.

Here, we present a framework that allows us to pin down the variability in BrC light-absorption properties. We hypothesize that BrC is comprised of black carbon (BC) precursors whose transformation to BC has not seen fruition during combustion. Depending on the combustion conditions, these BC precursors exhibit different maturity levels which dictate their light-absorption properties (k). The more mature are the precursors, the more absorptive (or BC-like) they are. This explains the aforementioned variability in k values reported in the literature: due to the chaotic nature of BrC-producing combustion, different measurements reported in the literature feature widely varying combustion conditions leading to different retrieved k values. More importantly, our hypothesis entails that BrC and BC lie on the same “optical continuum,” and carbonaceous combustion products can be represented as distributions along this continuum.

To validate this hypothesis, we performed controlled combustion experiments in which the combustion conditions (temperature and air/fuel ratio) were varied and the wavelength-dependent k was retrieved from real-time multi-wavelength light-absorption measurements at each condition. We used benzene and toluene, the inception of which during combustion marks the initial critical steps leading to BC formation, as model fuels. By varying the combustion conditions of these two simple molecules, we isolated BrC components with k values spanning the range of values reported in the literature for biomass-burning BrC, a clear evidence for the importance of combustion conditions in dictating BrC light-absorption properties. Specifically, the values we obtained for k at 550 nm (k_{550}) and its wavelength-dependence (w) ranged from $k_{550} = 0.005$ and $w = 8$ to $k_{550} = 0.3$ and $w = 0.4$. For reference, k_{550} and w of BC reported in the literature are approximately 0.7 and 0, respectively.

Our results unveil a continuum of optical bins defined by k_{550} and w pairs that progress from lighter BrC (small k_{550} and large w) to darker BrC (large k_{550} and small w) to BC. We stress that the darkest BrC we could isolate is optically more similar to BC than the lighter BrC components. This blurs the line between BrC and BC and challenges the wide-spread perception that BrC is negligibly absorbing in the mid- and long-visible wavelengths compared to BC and that its contribution to atmospheric radiative transfer is only important in the short visible and near-UV wavelengths.

9CA.5

Comprehensive Chemical Characterization of Brown Carbon Aerosols. Peng Lin, Lauren Fleming, Ying Li, Wing-Sy DeRieux, Julia Laskin, Manabu Shiraiwa, Sergey Nizkorodov, ALEXANDER LASKIN, *Purdue University*

Atmospheric Brown carbon (BrC) is a significant contributor to climate forcing. Understanding the climate effects of BrC, its sources, formation, and atmospheric aging mechanisms requires molecular identification of BrC chromophores and characterization of their light-absorption properties. Herein, we demonstrate an analytical method, which combines high performance liquid chromatography with three different detection technologies to comprehensively investigate UV/vis absorption spectra, chemical composition, and mass absorption coefficients of the individual chromophores in BrC aerosols. We highlight the applications of this methodology for the analysis of BrC in the samples collected from selected source emissions as well as ambient aerosols. The results show that BrC contains organic compounds of diverse molecular structures, polarities, and volatilities. Understanding their molecular identity requires multi-modal application of complementary ionization techniques in combination with high-resolution mass spectrometry. We demonstrate that optical properties of BrC and chemical composition of its chromophores depend significantly on the type of sources. The contributions to light absorption from different classes of chromophores such as aromatic carboxylic acids, nitro-phenols, polycyclic aromatic hydrocarbons (PAHs), and substituted PAHs are quantified, and their mass absorption coefficients are calculated. In addition, molecular speciation of aerosol components is used to estimate glass transition temperatures of individual components and viscosity of the resulting aerosol. The glass transition temperatures for BrC ranged from 254 - 286 K, suggesting that these particles may adopt an amorphous semisolid state at moderate relative humidity.

9CA.6

Brown Carbon at Three Platforms during the Actris-2 Experiment in Summertime in the Po Valley (Italy). STEFANIA GILARDONI, Angela Marinoni, Francesca Volpi, Douglas Orsini, Paolo Cristofanelli, Davide Putero, Matteo Rinaldi, Marco Paglione, Imad El Haddad, Minna Aurela, Julija Pauraite, Vidmantas Ulevicius, Dimitri Bacco, Vanes Poluzzi, Paolo Bonasoni, *ISAC-CNR*

Organic aerosol (OA) is a dominant component of atmospheric fine particles affecting air quality and possibly climate. Nevertheless, the optical properties of OA are far from being completely understood. Light absorbing OA, also known as brown carbon (BrC), accounts for up to 20% of anthropogenic aerosol warming [1]. In addition, recent measurements indicate that BrC short wavelength absorption can be larger than BC absorption, due to its vertical distribution [2]. Ambient observations indicate that different types of BrC are produced as primary pollutants, during combustion at low temperature and smoldering, or can be formed in the atmosphere through atmospheric processing.

We investigated OA optical, microphysical, and chemical properties in summertime at three platforms located in the Po Valley Italy, one of the European pollution hot-spots. Measurement platforms included Monte Cimone (remote mountain site, 44°12' N, 10°42' E, 2165 m asl), Bologna (urban background site, 44°31' N 11°20' E, 39 m asl), and San Pietro Capofiume (rural site, 44°39' N, 11° 37' E, 11 m asl). During the ACTRIS-2 experiment in July 2017 we deployed on-line high time resolution measurements (High resolution – Time of Flight – Aerosol Mass Spectrometer HR-ToF-AMS, and Aerosol Chemical Speciation Monitors ACSM), together with off-line OA UV-Visible light absorption measurements. Subsequent source apportionment analysis of OA spectra allowed for the quantification of OA components, whose mass absorption cross-sections (MAC) were calculated using bulk OA UV-Visible spectra.

OA accounted for more than 50% of fine particle mass at all the sites. OA MAC at 365 nm varied between 0.2 and 0.8 $m^2 g^{-1}$, in agreement with observations at locations dominated by secondary OA (SOA) [3,4]. Primary OA from fossil fuel combustion did not contribute to light absorption in the range 300-700 nm, while SOA components absorbed UV-Visible light, especially at short wavelengths. In agreement with literature data [4,5], aged SOA was characterized by higher MAC compared to fresh and local SOA. MAC dependency on OA oxygen content suggests that SOA at the low altitude sites was mainly from ageing of anthropogenic emissions. MAC values for specific OA types estimated by this study can improve models in describing the OA impact on climate.

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9CA.7

Field Measurements of Black and Brown Carbon Optical Properties from the 2017 Wildfire Season. KATIE FOSTER, Rudra Pokhrel, Matthew Burkhart, Shane Murphy, *University of Wyoming*

Biomass burning is known to have a significant impact on the Earth's radiative balance, and the measurement of aerosol optical properties from wildfires is both limited and bears a high degree of uncertainty. The University of Wyoming deployed a suite of aerosol instruments in a mobile laboratory to three different fires during the fall of 2017. A complementary suite of instruments for determining the optical properties of black and brown carbon consisted of: a multiwavelength Photo-acoustic Absorption Spectrometer operating at 405 nm and 660 nm in both dry and thermally denuded phases, two Cavity Attenuated Phase Shift – Single Scattering Albedo instruments at 450 nm and 660 nm, an Aerosol Mass Spectrometer, and two Scanning Mobility Particle Sizers. Single Scattering Albedo, Absorption Angstrom Exponent, Mass Absorption Coefficient, chemical composition, and volatility of organic aerosols are analyzed from multiple wildfires. The mobile lab sampled air from the Rice Ridge fire near Seeley Lake, MT as well as the Tubbs Fire of Santa Rosa, CA and the Lion Fire near Kernville, CA. The relationship between absorption enhancement by lensing, volatility, and aging will be discussed. Preliminary results suggest that low volatility organics are responsible for the majority of aerosol absorption at 405 nm.

9CA.8

Light Absorption by Organic Aerosol from Combustion and Pyrolysis of Fir in Southern China. RANRAN ZHAO, Yongming Zhang, Feng Wang, Qixing Zhang, *University of Science and Technology of China*

Biomass burning, including forest wildfires, residential heating and cooking, is an important source of light absorbing organic aerosols (OA). In this work, we performed a laboratory study of light absorption properties of OA from combustion of fir, which is a common tree species in southern China. Different moisture content of fir wood pieces were heated in air and nitrogen in a tube furnace under finely controlled temperature. Sampling filters were extracted with deionized water and methanol. The optical properties of water soluble organic carbon (WSOC) and methanol soluble organic carbon (MSOC) were analyzed and characterized by calculation of the absorption per mass, the imaginary part of the refractive index, and the Ångström absorption exponent (AAE).

We compared the results obtained from fir pyrolysis in nitrogen with those obtained from pyrolysis of oak and pine[1] and corn stalk[2]. The results show that the absorption per mass of WSOC obtained from fir pyrolysis generated at 270 ℃ is similar to that of oak , about 1.1m^2 / g at 360nm. In addition, the absorption per mass of MSOC obtained from fir pyrolysis at 360 nm is similar to that of oak and pine, but slightly higher than that of corn stalk. The fuel structure leads to the discrepancy. The AAE value of fir range from 7.2 to 7.8 in the range of 380nm to 460nm, similar to that of pine, oak and corn stalk.

The results also show the differences between OA from fir combustion in air and pyrolysis in nitrogen. OA produced by combustion of fir in the air has stronger light absorption in the UV region than that in the nitrogen. However, the result is opposite near the visible region. The differences could be attributed to the different thermal decomposition rate of volatiles during combustion and pyrolysis and the large amounts of black carbon (BC) generated during the combustion process. The details of this discrepancy will also be discussed.

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9IM.1

Modification of a Fine Condensation Particle Counter to Rapidly Measure Sub 3 Nanometer Atmospheric Clusters through Pulse Height Analysis. CHONGAI KUANG, *Brookhaven National Laboratory*

Atmospheric particle nucleation is an important environmental nano-scale process, with field measurements and modeling studies indicating that freshly nucleated particles can contribute significantly to the global population of aerosol and cloud condensation nuclei. Our understanding of atmospheric nucleation and its influence on climate, however, is limited, as few ambient measurements have been made of either the nucleation rate or the chemical composition of the freshly formed clusters, both of which are necessary to gain process-level understanding. Recent advances in the development of condensation particle counters (CPCs) have enabled the detection of gas-phase single molecules and molecular clusters down to 1 nanometer in diameter and below through the use of new working fluids and/or varying operating conditions. This new capability has enabled the direct measurement of aerosol nucleation from trace-gas precursors in both laboratory experiments and the ambient environment, providing information necessary to understand and constrain the nucleation mechanism. While there have been an increasing number of atmospheric cluster measurements from surface-based platforms, there have been very few measurements of the vertically-resolved ambient cluster size distribution from aerial platforms, which are needed to connect atmospheric nucleation with large-scale boundary layer transport processes. To address this measurement need, a commercial fine CPC (> 10 nanometers) has been modified to rapidly measure (~ 1 Hz sampling time resolution) the cluster size distribution (< 3 nanometers) through pulse height analysis. Characterizations of the modified CPC size-dependent counting efficiency and analysis of the resulting droplet size spectra to recover the sampled aerosol size distribution will be presented using high resolution electrical mobility classified ammonium sulfate aerosol and ambient aerosol.

9IM.2

Calibration and Ambient Measurements of Sub-3 nm Aerosols. HELINA LIPP, Eduard Tamm, Kalju Tamme, Kaupo Komsaare, Urmas Hõrrak, Heikki Junninen, *University of Tartu*

New particle formation (NPF) is a process where molecular clusters are formed from atmospheric vapours by condensation. The clusters can grow into larger particle sizes and act as cloud condensation nuclei. To investigate NPF in the ambient air it is necessary to use instrumentation that is capable of measuring the smallest formed particles around 1-2 nm in size. For this purpose, we used Airmodus A11 nano Condensation Nucleus Counter system (nCNC-system) containing the Condensation Particle Counter (CPC) in pair with Particle Size Magnifier (PSM) (Vanhanen et al. 2011). The foremost importance is on calibration of the instrumentation for accurate size separation. The instrumentation was calibrated in laboratory conditions and used for detection of nanoparticles in ambient conditions in the Station for Measuring Ecosystem-Atmosphere Relations (SMEAR) in Järvselja, Estonia.
SMEAR Estonia (http://smear.emu.ee/) is an environmental research and monitoring complex located in the hemiboreal forest of south-eastern Estonia at Järvselja, which can be described as a remote and rural site with low anthropogenic disturbances (Noe et al. 2015).

Our measurement system (A11 nCNC-system) was calibrated using tungsten nanoparticles, generated in a Carbolite STF tube furnace, where an alumina boat with a piece of tungsten wire was placed. Tungsten was evaporated at furnace temperature of 1100^{o}C, the vapour was excreted by the 1.5 l/min nitrogen flow through a nozzle and then turbulently mixed with cold clean air with flow rate of 1500 l/min. Nucleation process gave a polydisperse tungsten aerosol, particles were charged in a bipolaar charger and then a fraction with narrow distribution (quasy-monodisperse fraction) was selected by closed-loop DMA (Differential Mobility Analyzer). The A11 nCNC-system was operated in scanning flow mode together with aerosol electrometer as a reference instrument to find the detection efficiency and calibration coefficients. The calibration provides the PSM flow conditions for instrument detection of tungsten ions with diameters of 3 nm, 2.9 nm, 2.7 nm, 2.5 nm, 2.3 nm, 2.1 nm, 1.9 nm, 1.7 nm, 1.5 nm, 1.3 nm, 1.1 nm and 1 nm, respectively. We used diethylene glycol (DEG) as the working fluid of PSM.

Conducting the field measurements A11 nCNC-system was set up in a cabin so that the PSM inlet, which was a 51 cm long tube, was placed directly through the cabin wall for detection of nanoparticles in ambient conditions. In parallel with A11 nCNC-system the atmospheric aerosols and ions were monitored with NAIS (Neutral cluster and Air Ion Spectrometer) and EAS (Electrical Aerosol Spectrometer) for a complete size distribution of aerosols in hemiboreal forest. In the presentation the results from the ambient measurements will be shown and discussed in details.

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9IM.3

Comparison of Non-Radioactive Bipolar Charge Conditioners for Particle Ionization. SIQIN HE, Derek Oberreit,
Kanomax FMT, Inc.

Electrical mobility method has been widely used as a primary standard for size characterization of submicron aerosol particles, and it usually has a bipolar charge conditioner as an essential component because of the predictable steady-state charge distributions it can condition the particles with. Majority of bipolar charge conditioners used in aerosol researches are radioactive sources, such as Kr85, Po210, and Am241, because of their advantages in simple operation, stable performance, and low maintenance. However, as aerosol research extends from laboratory into real field environment, problems have arisen when using or transporting electrical mobility instruments because of the safety regulations over radioactive sources, and caused these instruments to be considered as unsuitable for field studies. To overcome the hurdle and extend the application of such characterization technique, alternative bipolar charge conditioning methods haven been developed using non-radioactive ionization sources, with the most representative two as corona discharge and soft x-ray.

To better understand the ionization performance of non-radioactive bipolar charge conditioners, three non-radioactive bipolar ionizers were evaluated and discussed in this study, with one based on corona discharge and two using soft x-ray. The ionizers were first evaluated and compared for their capabilities in establishing steady-state charge distributions with the same incoming particles from with or without pre-existing charges. Subsequently, effect of the (N·t) value on ionization efficiency was experimentally investigated at various residence time for each respective ionizer, and the results were compared to the Fuchs limiting sphere diffusion charging theory. Finally, fractions of singly charged particles exiting each charger were measured using monodisperse neutral particles within the size range of 5 to 100 nm, and the results were compared to theoretical values reported by Wiedensohler in 1988.

9IM.4

Improving Airborne Nanoparticle and Cluster Detection with the Butanol Based Laminar Flow Condensation Nuclei Counters Grimm 5.403 and 5.412. GERHARD STEINER, Manuel Orzan, Ina Nagler, Elena Petrakakis, Mirela Selimovic, Christian Tauber, Frank Tettich, *University of Vienna*

Over the last years, the size range of airborne molecular clusters (< 3nm) has become of highest importance in the field of aerosol sciences since it covers the initial steps of new particle formation in the atmosphere (e.g. Kulmala et al. 2013); therefore having a major climate relevant impact. Also, it was recently shown that a major fraction of traffic produced particles contributes to the sub 3nm size range (Rönkkö et al. 2017). Evidently, also the development of new instrumentation for the classification and detection of sub 3nm particles and clusters is an extremely emerging field.

The detection of charged aerosols and clusters in the size range below 3nm was investigated starting at the turn of the 19th to the 20th century (as reviewed e.g. by Flagan, 1998). The detection of electrically neutral aerosols in this size range is far more challenging and was most probably first made possible in the 1960’s by the development of a mixing type particle size magnifier (PSM) by Kogan & Burnasheva (1960).

Still, the state-of-the-art technique to detect electrically neutral particles by a single-particle count mode is based on the condensational growth of water or various alcohols. New types of condensation particle counters (CPCs) are designed as laminar flow type (e.g. Kuang et al. 2012), mixing type (e.g. Vanhanen et al. 2011) and expansion type (e.g. Winkler et al. 2008) CPCs. These instruments cover prototypes like the vSANC (Pinterich et al. 2016) and commercial products like the A10 Particle Size Magnifier (PSM) from Airmodus Oy and the Nano Enhancer 3777 from TSI Inc.

Accordingly, it appears, that for being able to detect low number concentrations of neutral sub 3 nm particles, one either needs to be expert in the field of the development of new instrumentation or one needs to invest money in a new commercial detector. Following the approach presented by Kangasluoma et al. (2015), this may not be necessary for some applications in laboratory measurements.

Here we present experiments with two n-butanol based CPCs (Grimm 5.403 and 5.412) that were operated with modified settings of their internal temperatures. We show the results of measurements with seed aerosols of different size and chemical composition and demonstrate improved detection of clusters down to 1.47nm (THA+; tetraheptylammonium ion).

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9IM.5

A Long-Term Stable High-Temperature Condensation Particle Counter for Application on Raw Automotive Exhausts.

MARTIN KUPPER, Michael Kügler, Alexander Bergmann, Martin Kraft, *CTR Carinthian Tech Research, Villach, 9524, Austria*

Introduction: Condensation nuclei counters (CNC) are widely used for measuring particle number (PN) concentrations. To both minimise the effort of aerosol preconditioning and eliminate possible condensation artefacts, CNCs operating at “high temperature” > 150 °C (HT-CNC) are of high interest for PN measurements, in particular in engine exhausts. Targeted research shows that key elements to realising such a long-term stably operable sensor are i) a suitable selection of wick and working fluid and ii) a special operation mode to prevent thermal degradation of the working fluid.

Experimental Methods: An experimental mixed-flow geometry HT-CNC setup was designed for application on raw automotive exhaust gas. To enable a loss-free long-term operation that is immune to thermal degradation of the working fluid, a special operation mode was developed that mixes a controlled fraction of the concentrated exhaust gas with an inert gas stream pre-saturated with the working fluid, a long-chained aliphatic hydrocarbon. This prototype was used for both, a fundamental proof of principle of an HT-CNC and various detailed studies. These studies include material tests of wick materials and a detailed examination of nucleation at HT-operation, investigating particles from ambient air, a GRIMM 7860 WOx-generator and a Jing 5201 miniCAST. The grown droplets were counted using specially developed fibre-optically coupled counting optics and sized using a dedicated static light scattering (SLS) setup. Finally, a calibration was performed and the HT-CNC was compared to a commercially available CNC (TSI 3775) using soot from the miniCAST.

Results: Tests with particles from ambient air and the WOx-generator proved heterogeneous nucleation in all tested wicking materials. The behaviour shows a strong dependence to the wick used since the (super-)saturation differs. Further it turned out that under normal operation the speed of degradation of the working fluid differs also from one used wick to another. Full prevention of the degradation of the working fluid was obtained by a special operation mode taking advantage of the mixed-flow geometry for all used material combinations. The examination of the grown droplets by SLS yielded reproducible droplet sizes at defined temperature gradients between saturator and condenser also at long-term operations. The comparison of the particle count to a TSI 3775 using soot from a Jing 5201 miniCAST showed a good agreement.

9IM.6

Measurement of Aircraft Engine Soot Emissions using the ESCOM (Engine Soot Compliance Monitor). Timothy Onasch, Richard Miake-Lye, Fred Bacon, Philip Croteau, William Brown, ANDREW FREEDMAN, *Aerodyne Research, Inc.*

We describe a new device, the Engine Soot Compliance Monitor (ESCOM), that provides a direct readout of the soot mass emission index (mass soot per mass fuel expended) from aircraft engines. The heart of this device is the CAPS PM_{ssa} monitor, operating at a measurement wavelength of 780 nm in order to avoid interference from emitted NO_2, which provides a highly accurate measurement of soot concentrations when used in conjunction with the soot mass absorption coefficient (MAC). Unlike other soot measurement instruments, it also provides a measurement of the single scattering albedo of the emitted particles. At the low single scattering albedo values found in aircraft engines (0.1-0.3), the CAPS PMssa monitor, which measures optical extinction and scattering, provides a highly accurate measurement of soot concentrations without external calibration. An embedded LiCor CO_2 monitor provides the carbon dioxide concentration which is used, along with known fuel composition to calculate the soot mass emission index. The monitor is capable of measuring soot concentrations at levels well below 1 $\mu g\ m^{-3}$ with a response time of 1-2 seconds. We will also present results from the Variant 2-3 campaigns, where emissions from an aircraft engine were measured over a range of operating conditions including different thrust levels and fuel composition. In these two campaigns, an older version of the monitor operating at 630 nm was used.

9IM.7

Experimental Results of a Novel Inverted Drift Tube with Diffusion Auto-Correction for the Characterization of sub 100nm Nanoparticles. XI CHEN, Md Minal Nahin, Carlos Larriba-Andaluz, *IUPUI*

A new mobility particle analyzer, termed Inverted Drift Tube(IDT), has been previously modeled analytically as well as numerically and proven to be a very capable instrument. The idea of the instrument was supported on the notion of existing shortcomings in previous instruments, i.e. diffusional broadening for high mobilities and inadequately low and fixed resolution (and hence not mobility dependent). The IDT, on the contrary uses two varying controllable opposite forces, a gas flow with velocity driving the particles, and a linearly increasing electric field that opposes movement. The effect of the linearly increasing field allows the IDT to overcome the diffusional broadening in the axial direction, constraining the charged nanoparticles and increasing the resolution several folds. Simultaneously, the use of two varying controllable forces allows controlled particle separation focusing on a given mobility. Hence, the separation ratio , is employed to determine the best possible separation for a given set of nanoparticles yielding a mobility dependent resolution which increases with particle size. Due to the system's need to operate at room pressure- in order to make it portable- two methods of capturing the ions have been developed; Intermittent Push Flow for a large range of mobilities, and Nearly-Stopping Potential Separation with very high separation but limited to a very narrow mobility range. The system has been extensively proven analytically and numerically showing a resolution increase of several fold over conventional DMAs attesting to the capability of the system.

To prove its validity, here we will show the construction, testing and results of an experimental prototype. The system consists of a set of concentric ring/electrodes arranged similarly to a drift type instrument with an electrostatic gate and an electrometer detector. An existing gas flow pushing the ions through the tube is carefully controlled through several flow meters, laminarizers and mechanical pumps while a linearly increasing electric field is controlled through a home-made software. Nanoparticles entering the system are subject to mobility separation and reach the detector at different times. The arrival time distribution does not provide a direct relation between signal and mobility (or diameter) so a dedicated software captures the signal as a function of the duty cycle, averages it over several cycles, and converts it into signal versus diameter. Preliminary data shows that enhanced separation is a function of your choice of separation ratio, maximum voltage applied and target mobility (or diameter) of choice. This focusing technology that allows the user to enhance separation for a given mobility precludes the use of instrument resolution as a reliable parameter and uses instead the chromatographic existing concept of resolving power to establish the degree of separation between two adjacent peaks. For example, two peaks with particles mobility of 2 and 2.3nm, respectively can now be separated several seconds.

9IM.8

Refinements of a Water-Based Condensation Particle Counter for Detection near 1 nm. Gregory Lewis, Steven Spielman, SUSANNE HERING, *Aerosol Dynamics Inc.*

Reported are refinements and further characterization of a water-based, condensation particle counter for particle detection near 1nm. This instrument operates at an aerosol flow of 0.3L/min, without use of a sheath. It employs a three-stage, laminar-flow growth tube with a cooled conditioner, followed by a short, warm initiator, and longer, cooled moderator. Operating temperatures are in the range of 1°-10°C, 80-95°C, and 10-20°C for the three stages, respectively. Walls are wetted throughout. Within the initiator stage, the transport of water vapor from the warm, wet walls is faster than the transport of heat, thus creating supersaturated conditions. The larger the temperature difference between the conditioner and initiator stages, the higher the supersaturation, and the smaller this particle size that is activated. The final moderator section reduces both water vapor content and temperature while maintaining supersaturated conditions.

As compared with the original prototype instrument, the new instrument has been designed to minimize the heat leak between stages, and to provide for much more rapid changes in operating temperatures. Operating temperatures of 1°C and 95°C are now attained within 3 minutes of start-up. Improvements in the temperature control of the final moderator stage eliminates the need for a water trap on the sample exit flow, as the flow is non-condensing at 20°C. As with the original prototype instrument, operation at an initiator-conditioner temperature difference of less than 84°C makes the instrument blind to ions from a bipolar ion. Calibration data show fifty percent efficiency cut-point varying from 1.5 nm to 2.0 nm depending on operating temperatures and aerosol type. The new system is self-contained with on-board pumps and water injection, and yet fits within the box of a standard water condensation particle counter. Unattended operation of two collocated units over a 4-day period yields a correlation coefficient R=0.99, and a regression slope of 1.02.

9LC.1

Towards High-Resolution Air Pollution Mapping: Fusing Mobile PM Measurements with Data from a Dense Low-Cost Sensor Network.

SARAH CHAMBLISS, Kyle Messier, Chelsea V. Preble, Julien Caubel, Ramon Alvarez, Brian LaFranchi, Melissa M. Lunden, Thomas W. Kirchstetter, Joshua Apte, *University of Texas at Austin*

Emerging techniques for measuring urban air pollutant concentration at high spatial and temporal resolution have the potential to greatly improve estimates of pollution exposure for urban populations. Two such techniques are (1) the deployment of a city-wide network of low-cost sensors and (2) mobile monitoring campaigns in which reference-grade instruments are routinely driven along all roads in a specified sampling area. Current research in the field seeks to answer how either technique may be optimally deployed to yield representative long-term exposure estimates with lower measurement density, and how a combination of techniques may provide complementary information to further improve exposure estimates. This study examines mobile and fixed black carbon (BC) measurements collected during an intensive two-month field campaign in summer 2017 in West Oakland, California. A dense network of 100 fixed sites was established within a 5 km^2 neighborhood. Time-resolved (1 min) BC measurements were collected using a novel low-cost sensor based on light absorption through a filter medium. Concurrent mobile measurements within this same domain were collected during a total of 341 sampling hours by two Google Street View cars specially equipped with photoacoustic extinctiometers measuring at 1 Hz.

The study compares 1 Hz and time-averaged on-road measurements to lower frequency measurements from nearby low-cost sensors to identify biases that may exist in either measurement method and to assess the comparative sensitivity of these measurements to localized emissions sources and short-term emissions events (e.g., vehicle plumes). On-road measurements include measurements taken while driving and collocation events, during which a Street View car was parked along a public street in proximity to a low-cost sensor. Thirty collocation sites were selected to provide an even distribution of sampling locations within the neighborhood and to represent a range of land uses and road types. Distances between parking and location sites ranged from 3 to 100 m. Measurements were collected for a minimum sampling duration of 5 minutes, with an average event duration of 15 minutes. The campaign included 183 full collocation events for a total duration of 47 sampling hours.

Preliminary analyses of the collocation data indicate modest correlation between BC concentration means calculated for the duration of each stop, and little to no correlation between one minute measurements. This loss of correlation with higher time resolution, along with high within-event variation and intermittent peaks observed in measurements taken at the parked car, may indicate the degree of increased sensitivity of on-road measurements to high frequency changes in emissions. Preliminary results also suggest that land use type may influence the level of agreement between a parked mobile monitor and off-road fixed site sensors. Further analysis will include comparisons with in-motion mobile measurements.

The findings of this study offer insight into how pollution monitoring campaigns may effectively integrate complementary sampling techniques to improve both the spatial and temporal resolution of exposure estimates. These findings may also suggest methods of improving the interpretation of mobile monitoring measurements to assess off-road urban exposure.

9LC.2

Development of the Scientific Payload for UAS Observation. FAN MEI, Jason Tomlinson, Albert Mendoza, Matt Newburn, Lexie Goldberger, Peter Carroll, Mikhail Pekour, Beat Schmid, *Pacific Northwest National Laboratory*

The aerosol measurements provided by various platforms are essential for contributing scientifically significant datasets to improve scientific understanding of earth system. With rapid growth in the variety of unmanned aerial system (UAS) platform and applications, the opportunity for UAS to provide high-quality atmospheric measurements continues to expand. However, limited aerosol UAS instruments are available, due to the weight, size and power constrains in UAS. The information about miniaturized instrument performance, characterization, and especially the compatibility with their sibling version used in aircraft are very rare. The ArcticShark owned by the U.S. Department of Energy (DOE) has the capability to measure a wide range of radiative, aerosol and cloud properties using a variable instrument payload weighing up to 46 kg. This work focuses on development of scientific payload in Department of Energy (DOE) Atmospheric Radiation Measurement (ARM) Aerial Facility (AAF). Several scientific payloads were tested based on the mission request. Aircraft-Integrated Meteorological Measurement System (AIMMS-30, Aven Tech.) is included in all the payload to provide the atmospheric state parameters and the aircraft condition. The aerosol payload includes printed optical particle spectrometers (POPS, Handix), and Aerosol Counting, Composition, Extinction and Sizing System (ACCESS, Brechtel). The operation of UAS version instruments compared with manned aircraft version were performed. In addition, the first UAS research flights data will be discussed.

9LC.3

Towards Improved PM2.5 Measurements Using a Low-cost Multi-sensor System. NUERAILI KUERBANJIANG, Meilu He, Suresh Dhaniyala, Clarkson University

In recent years, the use of low-cost particle sensors (LCPS) has become popular for air quality monitoring. Typically, these sensors are used in ambient monitoring after calibration against co-located FRM samplers. Such calibration efforts provide for site-specific conversion of sensor signals to PM. For a comprehensive understanding of the capabilities and limitations of these sensors, we conducted a series of tests with a range of popular OEM sensor units, and established the performance characteristics of the sensors under controlled conditions. We used size-classified particles from a differential mobility analyzer (DMA) and determined the concentration detection limit of LCPS for particles of varying compositions. The performance of the LCPS was established by comparison with number concentration measurements made using a condensation particle counter (CPC). The performance of the units was established as a function of temperature, humidity, and ambient wind-speed. We will present experimental results from our studies and identify sensor handling issues that are critical for accurate air quality measurements with these sensors.

9LC.4

Field Deployment Experience of Low Cost Smart City Air Pollution Monitoring Network. YU-TING CHEN, Chien-Wei Huang, Yeuh-Bin Wang, Shuenn-Chin Chang, Lung-Chi Lin, Chih-Ming Pao, Seng-Yong Lau, *Autotronic Enterprise Co., Ltd.*

In recent years, air pollution has become an emerging concern and high public awareness topic. The advance in sensor technology and low power long range communication protocol enabled the development and deployment low cost air pollution monitoring network. Such a network established a higher spatial and temporal density data collection system compare to traditional FEM method. In Cooperate with Environmental Protection Administration (EPA), Taiwan, this study present a field deployment experience of smart city air pollution monitoring network. A total of 700 sensing devices was installed on the street light in 4 different areas in Taiwan, covering industrial park, city traffic, small town and countryside. Install location is carefully selected, with 300~500 meters apart of each sensor, forming a grid network around the area of interest in order to achieve a better understanding of the propagation of the pollutant. The design consideration of the device is presented, which will measure the PM2.5, CO, NO2, O3, related humidity and temperature, and report the reading to a central server every 3 minutes. Prior to the deployment, lab evaluation compare the FEM equipment and field evaluation compare to standard EPA monitoring station was conducted. Two communication protocols, LoRaWAN and LTE CAT-1, is used in the deployment and the performance of each protocol is evaluated. During the course of more than a year of operation, long term degradation of the sensors is also examined. We also present the lesson learned from the deployment, negotiation experience with the local authority, real field deployment restrictions and problems, as well as the maintenance requirement in the paper. At last, in cooperate with the Environment Inspection Bureau, a few inspection checks were conducted based on the sensor data collected, and the result is presented.

9LC.5

Spatial Modeling of PM2.5 Concentrations Measured by a Low-Cost Sensor Network: Comparison of Linear and Machine-Learning Enabled Land Use Models. SAKSHI JAIN, Naomi Zimmerman, Albert Presto, *Carnegie Mellon University*

Low-cost sensors for PM2.5 and other pollutants can be widely deployed to characterize coupled temporal and spatial variations in concentration, inform human exposures, and disseminate information to the public. Many previous studies have characterized spatial patterns of PM2.5 by building land use regression (LUR) models from distributed filter samplers. These models can be generated with high spatial resolution, thereby producing estimates of long-term (e.g., annual average) spatial patterns of concentration. Deployment of low-cost PM2.5 sensors, which typically sample in real time, creates the possibility of time-resolved and/or real-time modeling of PM2.5 concentration surfaces. Additionally, since the low-cost sensors operate in real time, it may be possible to train models on a smaller number of sampling locations than in past studies that used integrated filter samples.

Our aim in this study is to develop spatial models for PM2.5 based on measurements collected by a network of low-cost PM2.5 nephelometers. We test two different models: LUR and a machine learning enabled land use model (land use random forest – LURF). LUR relates measured PM2.5 concentrations to land use variables (e.g., land zoning, population density, traffic intensity) using multi-linear regression. LURF uses the same basic structure and land use variables as LUR but uses random forests to link observed concentrations to land use variables. We expect LURF to outperform LUR because (1) near-source concentration profiles are not linear, and (2) LURF can resolve interactions between variables that are difficult to resolve in linear models, without overfitting.

Models were developed for daily average PM2.5 concentrations for periods spanning August 2016 through May 2017. PM2.5 data were collected from 15 different sites in Pittsburgh, Pennsylvania. We tested different combinations of sensors used for model training and validation. Land use variables included a set of 15 different classes of time-independent (e.g., building height) and time-dependent (e.g., wind speed) predictor variables.

We used both k-folds cross-validation and hold-out validation to evaluate model performance. For k-folds cross-validation, the training dataset for a subset of the 15 PM2.5 sampling sites was divided into 5 folds. Five different models were built, with each one using 4 folds (80% of data) for training and 1 fold for internal validation. The final model was an average across the set of models developed for each fold. For hold-out validation, we tested the model performance for sensors not used in model building. E.g., if the model was trained on 5 sampling sites, the remaining 10 were used to independently test the model. This validation tests model transferability both in space and time, as all sensors did not operate concurrently. We also performed a second, independent hold-out validation against a larger network of 35 additional PM2.5 sensors.

The LURF model significantly outperformed LUR model in cross validation and in most scenarios. With a testing window up to 13 weeks, the R-squared value for LURF model internal validation was above 0.75 and the Spearman rho value was above 0.9, for all cases that were tested.

LURF displayed greater temporal and spatial transferability than traditional LUR. A LUR model trained on 60 days of data from 10 sampling locations had R-squared value ~ 0.14. Whereas, similar training conditions in a LURF was able to predict concentrations at the remaining hold out sites (R-squared > 0.5).

9LC.6

Low-cost Sensor Calibration, Application, and Modification for Size Distribution and Refractive Index Measurements.

JIAYU LI, Jiaxi Fang, Tandeep Chadha, Benjamin Sumlin, Rajan K. Chakrabarty, Pratim Biswas, *Washington University in St Louis*

Compact low-cost sensors for measuring particulate matter (PM) concentrations are receiving significant attention as they can be used in larger numbers and in a distributed manner. Wang et al. (2015)[1] compared three types of popular low-cost PM sensor from Sharp, Shenyei, and Samyoung and summarized advantages and disadvantages of each sensor. To ensure accurate and reliable representation of PM mass concentrations, we calibrated the Sharp sensor with an optical method to study signal's dependence on composition and size distribution, which demonstrated why repeated calibration is needed for low-cost sensors[2]. Apart from laboratory studies, a networked low-cost PM sensor system has been applied in field measurements. They were deployed in households in Raipur, India to establish the spatiotemporal variation of PM concentrations[3]. From another study, in a woodworking shop, data collected by the networked sensor system was utilized to construct spatiotemporal PM concentration distributions using an ordinary Kriging method and an Artificial Neural Network model to elucidate particle generation and ventilation processes[4].

Almost all of the optical particle sensors make an assumption on the refractive index of the aerosols. As a result, the output of the current sensors could be inaccurate depending on the difference in optical properties of the calibration aerosols and measured aerosols. An improved system (OPSC) utilizes a three-wavelength particle counter coupled with accelerating nozzle time of flight measurements to measure the size distribution of the aerosol and to predict the material properties of the aerosol based on the refractive index of the aerosol. The three-wavelength particle counter measures the scattered light from a single particle at a time while the time of flight measurements utilize the peak intervals between successive detectors to measure aerodynamic size. These two measurements coupled together can be used to calculate the refractive index of the aerosol using the drag force and Mie Lorentz calculations. However, such calculations are computationally intensive. To mitigate the computation issue, machine learning algorithm was used to train the data and simplify the algorithm.

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9LC.7

Determination of the Size-Resolved Sampling Efficiency for a Commodity (AirBeam) PM2.5 Ambient Aerosol Sensor at a Background U.S. Continental Site. CHARLES STANIER, Nathan Janechek, Nathan Bryngelson, Megan Christiansen, *University of Iowa*

Commodity (also known as low-cost) aerosol sensors are widely accessible, provide real-time localized air pollution information, and can be used as educational tools for classroom and outreach applications. One such example of these sensors is the AirBeam from Habitatmap. The AirBeam is a portable, commodity ($250) sensor that can detect particles in the range ~0.5 – 2.5 µm and concentrations up to 400 µg m^{-3} at a resolution of 1 second.

While knowledge of site-specific calibration curves, interferences, accuracy, and precision information on commodity aerosol sensors is proliferating, detailed assessment of in-field size-selective sampling efficiency and dynamic response is rare.

Three AirBeam sensors were deployed co-located with SMPS and APS for 25 days during a summer 2017 measurement campaign in Zion, Illinois (north of Chicago along Lake Michigan). AirBeams were housed in tin enclosures with air vents to protect against the weather. Mass concentration, temperature, and humidity were recorded every second by the AirBeams and uploaded to the crowdsourced website. The three AirBeams had good reproducibility with concentrations similar to each other.

Reference instruments measured the aerosol size distribution every 2 minutes, and when used to estimate aerosol mass, PM2.5 concentrations ranged from 1 to 20 µg m^{-3}. The AirBeams, when averaged to the same time basis, were highly correlated, and able to reproduce short-duration peaks in aerosol concentration. The correlation coefficient (r) at 2-min time resolution with the reference instruments was 0.95. However, the AirBeams reported lower concentrations (0.1 – 12 µg m^{-3}) using the manufacturer calibration curve (counts to mass), and the average slope between the commodity and reference instruments for PM2.5 mass was 0.59. Correlation persisted even to very low concentrations in the 1-3 µg m^{-3}, however, the slope varied significantly with concentration.

We will discuss the construction of a size-resolved effective sampling efficiency for the AirBeam, and explore the degree to which it may be generalized to other locations. Our technique will rely on comparison to a reference aerosol size distribution, measured from 1 nm to 2.5 microns every 2 minutes, together with twice-daily organic and inorganic PM2.5 chemical speciation and collocated gravimetic PM mass and meteorological variables. We will investigate if the sampling efficiency varies with relative humidity, temperature, solar radiation, Aeronet aerosol optical properties, black carbon fraction, or other aerosol chemistry factors, and thereby assess the transferability of our efficiency model to other sites.

A stand-alone CPC measuring with 1 second time resolution and known dynamic response for the inlet and instrument, will be used to assess the effective dynamic response for the AirBeams and calculate an effective time-constant for the AirBeam samplers in their housings. This will likely vary with wind speed and that relationship will be evaluated.

The AirBeam uses a Shinyei PPD60PV-T2 sensor which measures light scattering for a single bin which is converted to an estimated mass concentration using a calibration fit developed from outdoor urban aerosols. A corresponding Android device is used to visualize, record, and upload measured data to a crowdsourced website that maps the spatial and temporal resolved data. Previous evaluation of the AirBeam in a laboratory environment at high loadings indicated good reproducibility between sensors and poor correlation compared to traditional instruments.

The AirBeams observed good correlation for ambient outdoor PM2.5 concentrations although concentrations are lower than well-established methods. The AirBeam and AirCasting system provide an easy way to upload and retrieve the sensor data, but frequent Bluetooth connection drops between the Android device and AirBeam occurred.

9LC.8

Ambient and Laboratory Performance Assessment of Plantower PMS Low-Cost Particulate Matter Sensors. TOFIGH SAYAHI, Kerry Kelly, *University of Utah*

Low-cost particulate matter (PM) sensors are becoming more widely available and are being increasingly deployed in ambient and workplace environments due to their low cost and ability to provide highly resolved spatial and temporal PM data. However, these inexpensive sensors have limitations and need to be characterized for the conditions of use. This study evaluated two models of a low-cost light-scattering PM sensor (the Plantower PMS 3003 and 5003) under controlled laboratory and ambient conditions. An aerosol chamber was designed and used to assess laboratory performance of 153 Plantower PMS 3003 sensors using two different types of particles, representing dust and secondary aerosols. This chamber is capable of providing uniformly distributed particle concentrations to eight low-cost sensors and a reference instrument. The ambient sensor evaluation occurred at two state monitoring stations located in urban residential areas in Salt Lake City, UT and included elevated PM levels caused by cold air pools, fireworks and wildfires. In addition, 50 sets of two co-located Plantower PMS 5003 sensors (dual sensors) deployed in different parts of Salt Lake City, UT and were evaluated over a period of 3 months in the winter of 2017 to investigate the inter-device agreement of the sensors during periodic episodes of high PM levels associated with several cold air pool events. The laboratory and ambient assessments allow us to evaluate the performance of the low-cost sensors in terms of precision and accuracy of measurements, limits of detection, drifts and linearity of the response. The laboratory results show high correlations between the reference instrument (TSI DustTrakII) and the PMS 3003 $PM_{2.5}$ readings (R^2>0.978). The long-term ambient evaluation of the PMS 3003 also showed high inter-sensor correlations (R^2>0.975) and great agreements with FEMs (R^2>0.882). In addition, comparing the slopes of the linear relationships for the dual sensors showed that 66% of these slopes agreed within 15% of each other.

9MG.1

Secondary Organic Aerosol Formation from Urban Sources: Current Understanding and New Results from WINTER in the NE US. JOSE-LUIS JIMENEZ, Jason Schroder, Patrick Hayes, Joost de Gouw, Viral Shah, Lyatt Jaegle, Pedro Campuzano-Jost, Douglas Day, Benjamin A. Nault, *University of Colorado-Boulder*

Secondary organic aerosols (SOA) are particle-phase species formed from chemical reactions of gaseous organic compounds. SOA formed from urban sources (i.e. from emissions within urban areas) is a substantial contributor to particle concentrations in polluted regions, with important impacts on human health, visibility, and climate. In this presentation we will summarize recent progress on the understanding of SOA formation from urban sources, and to point towards the areas that require further research. We will also present results from the WINTER 2015 field study in the NE US, which was one of the first studies to characterize urban SOA with an advanced aircraft payload in winter.

The amount of SOA formed from urban sources can be quantitatively characterized and compared across different locations using techniques that normalize for the effects of changing emissions, dispersion, and photochemical age, such as the ratio of excess OA to excess CO (above their respective background levels), or the regression slope of SOA to Ox (O3 + NO2). Results from many developed world megacities (e.g. Los Angeles, Paris, Tokyo, Mexico City, NE US) are quite similar, highlighting the global importance of SOA from urban sources. A timescale of 1 day or less for formation of urban SOA is consistently observed. Results for smaller urban areas can be ambiguous if the signal-to-background ratios are small. Three-dimensional models should be evaluated using these same techniques, as if their results were experimental data. Merely comparing measured to modeled SOA concentrations can lead to very erroneous conclusions due to differences in emissions, dispersion, and photochemical aging (e.g. Woody et al., ACP, 2016).

SOA formation in WINTER was consistent with summer studies, once differences in OH are accounted for. SOA formed from anthropogenic volatile organic compounds (VOCs) emitted in urban areas is important, while SOA formed from biogenic VOCs emitted within the urban area is typically a very small contributor. However, biogenic SOA advected into urban areas from sources outside of it can be an important and even dominant contributor to urban SOA concentrations. Pre-2007 models of urban SOA are low by about an order-of-magnitude. This huge urban SOA underestimation still affects recent versions of widely-used models, e.g. CMAQ v.5.0.2 and the non-volatile POA version of GEOS-Chem v10. Vapor wall losses in Teflon chamber SOA experiments affected older SOA models, and contributed to this underprediction. The most commonly used Volatility Basis Set (VBS)-type models produce too much SOA and do so much too slowly, compared with observations. There is strong evidence that urban VOCs and semivolatile and intermediate volatility species (S/IVOCs) are both important as SOA precursors. Updated models still predict SOA formation that is too slow compared to observations, suggesting the importance of faster chemical pathways such as autoxidation.

Motor vehicles are significant, but probably no longer dominant contributors to urban SOA. There are indications that SOA from cooking emissions may also be important, which would help explain the substantial non-fossil fraction of the SOA from urban precursors. Solvents, personal care products, and other volatile chemical products (VCPs) are also likely important (McDonald et al., Science, 2018). Both cooking and solvents/PCPs will likely become more important in the future as vehicle emissions continue to be aggressively reduced, and more research on SOA formation from both sources is urgently needed. SOA from urban sources is poorly characterized for megacities in the developing world.

9MG.2

Airborne Fine Particulate Matter in the Subway System of the Megacity of São Paulo. ADMIR CRÉSO TARGINO, Patricia Krecl, Julián Felipe Segura, *Federal University of Technology*

Subway systems are efficient mass transportation modes, especially in megacities with neighborhoods separated by long distances. Nevertheless, below-grade stations are enclosed spaces that facilitate the build-up of concentrations of airborne particulate matter (PM) entering from both the outside sources and generated by the abrasion of rail tracks, wheels and brake pads. Despite spending only 7-10% of the day within transport microenvironments, urban dwellers can be highly exposed to airborne PM while commuting. The subway system of the megacity of São Paulo comprises five lines, covers 71 km, serves 64 below- and above-grade stations and transports on average 3.7 million passengers daily on weekdays. The system operates electric trains with steel wheels rolling on steel tracks. For the first time, concentrations of black carbon (BC) and particle number (PN) were monitored in the city's subway system with a high temporal resolution using hand-held condensation particle counters (a P-Trak and a CPC model 3007, TSI, USA) and aethalometers (AE51, Aethlabs, USA). The monitoring was conducted on the green and yellow lines simultaneously during one week in August 2017. The AE51 and the particle counters were operated with temporal resolutions of 10 s and 1 s, respectively. The sampling protocol followed a pattern of boarding and disembarking at each station up to the end of the lines when the researchers returned to complete the loop. Because the smallest detectable particle size of the P-Trak was 20 nm and of the CPC was 10 nm, we collocated the instruments for about one hour before each sampling session to extract linear regression equations using the CPC measurements as reference ($R^2 > 0.90$). Thus, the P-Trak measurements were harmonized by using the slopes and offsets found in the intercomparison. Overall, the concentrations increased rapidly when the researchers disembarked and spiked as trains approached, with values consistently larger at the platforms than in the trains. The average BC and PN concentrations on the yellow line were 11.3 µg/m^3 and 37.000 pt/cm^3 at the platforms and 10.1 µg/m^3 and 30.400 pt/cm^3 in the trains, with maximum values of 241 µg/m^3 and 287.000 pt/cm^3 at República (a below-grade station in São Paulo's city center). The average BC and PN concentrations on the green line were 9.1 µg/m^3 and 22.200 pt/cm^3 at the platforms and 7.3 µg/m^3 and 18.000 pt/cm^3 in the trains. Despite the larger particulate concentrations at the platforms, on some occasions BC and PN did not follow each other and were overall poorly correlated, with maximum R^2 of 0.3 on the green line and 0.4 on the yellow line. This is likely to be associated with the generation of metallic particles by the wheel−rail friction, which may not have absorption properties at the wavelength of 880 nm used by the AE51, but can be detected by the particle counters. Comparison between concurrent BC measurements on Paulista Avenue (a thoroughfare with 6.400 vehicles/h at peak hours) and the nearby below-ground Trianon-MASP station showed that the average concentrations were 7.2 and 11.1 µg/m^3 at street level and at the platform, respectively. Our results revealed that the concentrations of fine PM in the subway system of São Paulo were large and highly variable with substantial differences in the train and at platforms. We will explore details of the spatial distribution of PM on both lines and identify features in the design and location of stations which may drive the differences in concentrations.

9MG.3

The Impact of Mixing State and Size-resolved Hygroscopicity of Urban Aerosols on CCN Activity in Seoul, Korea. NAJIN KIM, Minsu Park, Seong Soo Yum, Hye Jung Shin, Jong Sung Park, Joon Young Ahn, *Yonsei University*

Studies for atmospheric aerosol properties and their impacts on global climate change and air quality has been conducted steadily. Especially, hygroscopic properties of aerosols, which describe how well aerosols interact with water vapor in sub- and supersaturated conditions, are considered to be particularly important as they are closely related to cloud condensation nuclei (CCN) activity that is connected to aerosol-cloud interaction problems. Although many field campaigns for examining aerosol properties have performed around the world, observational data in various regions is still needed as aerosols have diverse sources and temporal-spatial distribution.

As an effort to add such observational data, field campaigns with a comprehensive set of measurements were made during May-June 2015 (Megacity Air Pollution Studies, MAPS-Seoul) and 2016 (KORea-United States Air Quality study, KORUS-AQ) in Seoul, highly urbanized area where various anthropogenic sources exist. Ground-based measurements for aerosols included aerosol (condensation nuclei, CN) and CCN number concentrations (N_{CN} and N_{CCN}), aerosol size distribution and aerosol chemical composition. Especially, size-resolved aerosol hygroscopicity with four dry diameters were measured by hygroscopic tandem differential mobility analyzer (HTDMA).

In Seoul, average N_{CN} (>10nm) was about 11000 cm^{-3} for KORUS-AQ which was slightly lower than those of MAPS-Seoul and showed diurnal pattern peaking at morning and midday. Unlike N_{CN} , both of N_{CCN} at 0.6% supersaturation had little diurnal variation. κ values which are obtained from HTDMA results and represent aerosol hygroscopicity, ranged 0.17-0.27 (MAPS-Seoul) and 0.11-0.24 (KORUS-AQ). Aerosols were classified into three types based on mixing state and hygroscopic growth factor (GF): Type 1 (externally mixed aerosol), Type 2 (Internally mixed and growth aerosol) and Type 3 (Internally mixed and non-growth aerosol). During both of campaign periods, small (30nm and 50nm) and large (100nm and 150nm) particles have different diurnal pattern of aerosol types as well as aerosol hygroscopicity. Significant portion of externally mixed particles and their distinct diurnal pattern implies that mixing state of aerosols has to be considered when prediction of N_{CCN} is performed. Predicted N_{CCN} with two assumptions (internal and external mixture) were calculated based on size-resolved hygroscopicity data and then compared with measured N_{CCN} . In practice, better results of predicted N_{CCN} with externally mixture assumption were obtained rather than simple internal mixture assumption. Comparison of campaign results with long-term observational data and detailed analysis will be shown at the conference.

9MG.4

Seasonal Characterization of Organic Nitrogen in Atmospheric Aerosols Using High Resolution Aerosol Mass Spectrometry in Beijing, China. WEIQI XU, Yele Sun, Qingqing Wang, Wei Du, Jian Zhao, Xinlei Ge, Tingting Han, Yingjie Zhang, Wei Zhou, Jie Li, Pingqing Fu, Zifa Wang, Douglas Worsnop, *Inst. of Atmospheric Physics, Chinese Academy of Sciences*

Despite extensive efforts to characterize organic nitrogen (ON) in atmospheric aerosols, knowledge of the sources and processes of ON in the megacity of Beijing is still limited, mainly due to the complexity of ON species and the absence of highly time-resolved measurements. Here we demonstrate the applications of Aerodyne high-resolution time-of-flight aerosol mass spectrometer combined with positive matrix factorization in characterization of ON in submicron aerosols. Our results show that the average nitrogen-to-carbon ratios (N/C) vary from 0.021 to 0.028, and the average ON concentrations range from 0.26 to 0.59 μg m^{-3} during four seasons in Beijing. ON accounts for 7-10% of the total nitrogen (TN) on average, yet the sources vary differently across different seasons. We found that 56-65% of ON was secondary during three seasons except winter when 59-67% was related to primary emissions. Particularly, more oxidized secondary organic aerosol contributes the dominant fraction of ON (39-44%) in spring, summer and autumn, while biomass burning is a more important source of ON in winter (23-44%). These results are consistent with the better positive correlations between N/C and oxygen-to-carbon ratio, a surrogate of organic aerosol aging, during these three seasons than that in winter. N/C also shows a clear increase as a function of relative humidity during all seasons, suggesting that aqueous-phase processing likely played an important role in formation of nitrogen-containing compounds. In addition, the uncertainties and limitations in quantification of ON with aerosol mass spectrometry are illustrated, particularly, ON could be underestimated by ~20 – 42% by ignoring the fragment contributions in NH_x^+ and NO_x^+.

9MG.5

Investigation of Organic Aerosol in Delhi, India, using an Extractive Electrospray Ionization Time-of-Flight Mass Spectrometer (EESI-LTOF). Varun Kumar, Deepika Bhattu, Yandong Tong, Veronika Pospisilova, Giulia Stefenelli, Amelie Bertrand, Roberto Cassotto, Rangu Venkata Satish, Pawan Vats, Urs Baltensperger, Dilip Ganguly, Neeraj Rastogi, S.N. Tripathi, Andre S.H. Prévôt, JAY G. SLOWIK, *Paul Scherrer Institute*

The densely populated Indo-Gangetic Plain is subject to extremely high particulate matter (PM) concentrations during winter, which significantly affect radiative forcing, increase mortality rates, and cause other deleterious effects on human health. Pollution reduction efforts are hindered by the lack of consensus on the dominant factors governing PM concentrations, particularly the relative importance of specific sources, primary vs. secondary aerosol, and secondary aerosol formation pathways. In particular, investigation of secondary organic aerosol (SOA) sources and formation processes has traditionally been hindered by the reliance of conventional online instrumentation on thermal desorption and/or hard ionization, which destroys much of the chemical information needed for source and process identification. The recently developed extractive electrospray ionization long-time-of-flight mass spectrometer (EESI-LTOF) overcomes these obstacles by continuous sampling of aerosol into a spray of charged droplets (100 ppm NaI in 50:50 water/acetonitrile) generated by a conventional electrospray probe. Soluble components are extracted, the droplets are gently evaporated, and the intact organic molecules are detected as charged adducts with Na+, with the observed signal proportional to mass concentration. Here we use the EESI-LTOF to investigate SOA sources and formation processes in the Indian capital city of New Delhi during a field campaign from January to March, 2018.

New Delhi is home to nearly 19 million people and routinely experiences very poor air quality during the winter due to a combination of a low boundary layer and emissions from a complex array of sources, including vehicle traffic, domestic wood and coal heating, cooking emissions, and uncontrolled combustion activities (e.g. trash burning). The EESI-LTOF was deployed on the campus of the Indian Institute of Technology Delhi, an urban background site approximately 10 km south of the city center. Supporting instrumentation onsite included an Aerodyne high resolution long-time-of-flight aerosol mass spectrometer (L-ToF-AMS), as well as measurements of organic gases (by proton transfer reaction mass spectrometry), trace elements, and optical absorption. SOA sources and formation are characterized by investigation of process-specific tracer ions in the EESI-LTOF mass spectra identified in previous chamber and field campaigns, as well as by positive matrix factorization (PMF) utilizing the Source Finder (SoFi) interface for the multilinear engine (ME-2). We assess the importance of the major secondary sources governing SOA formation, their likely formation pathways, and implications for optical and health-related properties.

9MG.6

Gradients in Concentration and Composition of Sub-Micron PM in a Coastal American City: Downtown Street Canyon Dominates a Large Area Emission Source in Port of Oakland CA. RISHABH SHAH, Ellis Shipley Robinson, Peishi Gu, Joshua Apte, Albert Presto, *Carnegie Mellon University*

We deployed an Aerodyne HR-ToF-AMS along with a suite of other gas and particulate measurement instruments in the Carnegie Mellon University mobile laboratory. Repeated drives were performed over an urban domain in Oakland, CA between 10th July and 2nd August, 2017. Oakland has a somewhat unique land-use feature in that a 1 km^2 downtown, a 6 km^2 residential district as well as one of the largest US ports (5 km^2) all lie within a short spatial transect of 4 km. Our objective was to quantify (a) spatial variations in non-refractory chemical components of PM_1 to identify local emission hot-spots and (b) contribution of fresh versus photochemically processed emissions to the local PM_1. The campaign-median mass-based non-refractory chemical composition of PM_1 was 58% organic, 24% sulfate, 9% nitrate, with other species making up the balance.

Mobile sampling data were aggregated using artificial "magnets" located every 200 m along all city streets. Each AMS sample, once aligned in time with GPS co-ordinates, was assigned to the nearest magnet for averaging. Spatial analysis and magnet creation were done in Q-GIS software. Approximately 70% of the magnets in the domain are represented by measurements on more than 15 unique days, which means that the data should be representative of seasonal- or even annual-average spatial patterns. Bias in temporal-spatial coupling of PM_1 concentrations was avoided in two ways: first, we varied the sampling route on each day, so that certain areas were not systematically sampled in morning versus afternoon. We also calculated a time-series-based estimate of background concentrations by fitting a spline to the 5th percentile of every x min of smoothed data. We observed the diurnal stability of the estimated background on a few days and its sensitivity to the value of x. We found that if x is chosen to be too small (e.g., 20 min), or too big (e.g., 9 hours), most of the spatial variability gets underestimated or overestimated, respectively. However, for x = 90, 120 and 240 min, the estimated background levels and trends remain stable. For each "magnet", background levels were subtracted from raw data and the remaining "above background (AB)" values were used for calculating a temporal average (μ_{AB}) and standard deviation (σ_{AB}).

We find that inorganic PM_1 components like sulfate and ammonium are spatially stable, whereas PM_1 organics are highly spatially variable. For instance, average organic aerosol concentrations in downtown Oakland are consistently higher ($\mu_{AB} = 2.2\ \mu gm^{-3}$) as well as internally spatially variable ($\sigma_{AB} = 1.8$) as compared to the relatively large area source, the port of Oakland ($\mu_{AB} = 1.4\ \mu gm^{-3}$, $\sigma_{AB} = 1.1$) as well as the largely residential West Oakland neighborhood ($\mu_{AB} = 1.1\ \mu gm^{-3}$, $\sigma_{AB} = 0.8$). Further, by plotting normalized organic signals of source-specific marker ions m/z 55 (indicative of cooking emissions) and m/z 57 (indicative of vehicular emissions), we find their relative abundances strongly influenced by time of day. While m/z 57 signal dominates during morning traffic rush, it is rapidly overwhelmed by m/z 55 after ~ 10 AM. This finding not only confirms the recently elsewhere investigated influence of cooking-induced emissions on local urban air quality, but also has implications for human health and exposure given that these elevated signals are found in areas and times of high human presence in urban locations. Next analyses include source-apportionment using positive matrix factorization to identify the distinct chemical source profiles (fresh and relatively aged components) and their relative contribution to local urban PM_1 hot-spots.

9MG.7

PM1 Chemical Characterization in 2015, South of Mexico City, with an Aerosol Chemical Speciation Monitor. DARA SALCEDO, Harry Alvarez-Ospina, Oscar Peralta, Telma Castro, *National University of Mexico*

The Mexico City Metropolitan Area (MCMA) is the largest megacity in North America with over 20 million people in 1500 km2. Historically, the MCMA has suffered of bad air quality by ozone and particulate matter (PM), causing severe health effects on its population. However, very few studies regarding the chemical composition of particles have been done. The last large one was held during the MILAGRO campaign in 2006 (Molina, et. al., 2010. Atmos. Chem. Phys., 10, 8697–8760) which included several sites north of Mexico City. A more recent study published in 2017 (Guerrero, et al., 2017. Atmosfera, 30, 243-273) discussed how has the chemical composition of PM in the north of the MCMA changed from 2006 to 2014. In this presentation, we will describe the chemical composition of PM1 in a site south of Mexico City using an Aerodyne Aerosol Chemical Speciation Monitor (ACSM) from January 19 to March 19, 2015. The organic fraction of PM1 was analyzed using the Positive Matrix Factorization (PMF) model in order to deconvolve it into distinct factors of different origin. The ACSM data will be compared with criteria air pollutants and black carbon concentrations, as well as meteorology parameters. Differences between the chemical composition of particles in the north and south of the city will be discussed in relation to the PM sources found in each site.

9MG.8

Exploring the Chemical Composition of Gas and Aerosol Phase Measurements from FIGAERO-ToF-CIMS in Beijing Using Positive Matrix Factorisation. ARCHIT MEHRA, Manjula Canagaratna, Stephen Worrall, Asan Bacak, Thomas Bannan, Michael Priestley, James Lee, Freya Squires, James Hopkins, Rachel Dunmore, Jacqueline F. Hamilton, Eloise Slater, Lisa Whalley, Yele Sun, Pingqing Fu, James Allan, Carl Percival, John Jayne, Douglas Worsnop, Hugh Coe, *University of Manchester*

Globally, air quality in megacities such as Beijing is of increasing interest due to its impact upon health. With a complex mixture of emission sources, it is challenging to understand the key drivers of the pollution; however it is vital to do so for effective and relevant policy implementation. The Air Pollution and Human Health Beijing (APHH-Beijing) project is a joint UK-China collaboration which aims to identify both the concentrations and sources of urban pollution in Beijing and people's exposure to this pollution in order to further understand its impact upon health. Within this project, AIRPOLL-Beijing aims to identify sources and emissions of air pollutants while AIRPRO focuses on air pollution processes in Beijing. Two intensive periods of measurement in Beijing were carried out in November-December 2016 and May-June 2017. A wide range of instrumentation was deployed at the Institute of Atmospheric Physics, an urban measurement site in North Beijing between the third and fourth ring roads. Here we present observations from the FIGAERO-ToF-CIMS which enables simultaneous detection of the molecular composition of the gas and particle phases through use of a Filter Inlet for Gases and AEROsols (FIGAERO) coupled to a time of flight chemical ionisation mass spectrometer (TOF-CIMS). Observed species are detected as adducts with the reagent ion, Iodide, which is highly sensitive and selective for multifunctional oxidised organic molecules. Positive Matrix Factorisation (PMF) is applied to this data to probe the relative contributions of different sources and processes to the pollution in Beijing and how these source profiles vary temporally during the campaigns. The analysis has been able to identify factors with varying volatility in the aerosol phase, alongside factors potentially relating to biomass burning, vehicular emissions and secondary processes.

9WA.1

Towards Better Particle Characterization in Industrial Workplaces. TORUNN ERVIK, Stephan Weinbruch, Dag Gunnar Ellingsen, Yngvar Thomassen, Balázs Berlinger, *National Institute of Occupational Health, Norway*

Exposure to airborne particulate matter (PM) is a major risk factor for development of respiratory and cardiovascular diseases. Epidemiological and experimental studies have shown that particle size and physical and chemical properties of the PM are of importance, with possible increased toxicity of the smallest particles. Many industrial workers are exposed to agglomerates/aggregates composed of primary ultrafine particles (<0.1 µm). These primary particles are unintentionally formed, e.g. in thermal processes used in the production of metals/alloys, by welding and by mechanical grinding of clinker in cement factories.

The aim of the present study is to characterize the PM in workplace air during various industrial processes with regard to particle size distribution, morphology, chemical composition and solubility/bioavailability. PM formed in recycling and casting of precious metals, production of cement, aluminum, silicon, silicon carbide, ferroalloys (silico- and ferromanganese, ferrosilicon) and nano zinc metallic powder; in different welding techniques and other hot processes such as plasma and thermal cutting and air carbon arc applications are under characterization.

The applied sampling and analytical methods include the use of personal and stationary cascade impactors for subsequent characterization of the particle fractions by gravimetric analysis, electron microscopy (SEM, ESEM, TEM) and atomic spectrometry (ICP-OES, ICP-MS).

In this presentation the characteristics of PM present in workroom air during production of manganese alloys and silicon carbide with respect to particle size (mass and number) distribution, morphology, chemical composition and solubility/bioavailability will be discussed.

9WA.2

A Novel Approach for Investigating Workplace Ultrafine Particles Respiratory Deposition. WEI-CHUNG SU, Yi Chen, *University of Texas Health Science Center at Houston*

Ultrafine particles (UFPs) in workplace has been and continues to be an important occupational health concern. Many workplace operational processes, such as welding and combustion, are known to generate UFPs in workplace. The inhalation and the consequent deposition of UFPs in the worker's lower airways could lead to adverse health effects. Therefore, investigating the deposition of UFPs in the human respiratory tract is vital from the viewpoint of occupational health. Conducting experiments on UFP respiratory deposition using human airway replicas can provide valuable information of the deposition pattern and deposition efficiency of the inhaled UFPs. However, due to the limitations of the current experimental approach, it is difficult to conduct UFP respiratory deposition experiments in the human lower airways. As a result, the nature of UFP deposition in the human airways remains not well understood. To fill this gap, a novel experimental method has been developed in this study to measure the deposition of UFP in the lower respiratory tract. A hollow human tracheobronchial airway replica down to the 10th lung generation was made by a 3D printer. The tracheobronchial airway replica along with a human oral airway replica were used to build a simplified airway system. With the assistance of two GRIMM SMPS+C systems, and a series of trimmed airway replicas (modified based on lung generations), UFP deposition in individual lung generation of the tracheobronchial airways could be directly and systematically measured by the experimental approach developed. The deposition data acquired can be applied to estimate the UFP inhalation dosimetry for UFP related workers, and used for validating relevant numerical simulation data.

9WA.3

Effective Density Determination For Workplace Real-Time Monitoring of Ultrafine Aerosols Using An ELPI+. LOÏC WINGERT, Yves Cloutier, *IRSST/ETS*

Ultrafine particles aerosols (UFPs) can be found in many workplaces depending on workers activity or industrial processes (combustion, mining, grinding…). Because of health issues linked to the UFPs, workplace air monitoring is performed by Occupational Health and Safety agent. Many aerosols properties are often needed to assess their toxicity or to fully describe them such as particle size distributions, total concentrations or the size-resolved particles chemical composition. Furthermore, time-resolved and time-weighted averages values are also of interest. Therefore, it is often necessary to use simultaneously several devices (SMPS, filter samplings, cascade impactor…) leading sometimes to issues of space and weight-carrying.

The ELPI+ (Electrical Low Pressure Impactor, Dekati®) could solve this issue but to be operated properly the particles effective density of the particles need to be known. The ELPI+ has the advantages to be able to collect aerosols on removable substrates for further gravimetric and chemical analysis. The ELPI+ is equipped with an electrometer for each impaction stage that gives a time-resolved number particle size distributions (NPSD). As it has been said, for these NPSD to be correctly calculated, one needs to know the particle effective density. In the ideal case of spherical and non-porous particles, this density is equal to the raw material density. Unfortunately, almost all of the time workplace aerosols are unsteady mixtures of irregularly shaped and porous UFPs whose effective density is decreasing with particle diameter. To determine this size-dependent effective density, tandem analysis described in the literature (DMA-ELPI+, DMA-APM…) can be used. Although these methods are precise and adapted to laboratory experiments, they present the disadvantages to be time-consuming and unable to monitor quick changes in aerosols composition that occur frequently in workplaces. Furthermore, it would mean to carry another heavy and expensive device with the already cumbersome ELPI+. Because of these difficulties, people don't use ELPI+ in the workplaces for real-time measurements or assume a unit density leading to significant errors.

To overcome these issues, we developed a method based on: (1) the synchronous use of an ELPI+ and a hand-held condensation particles counter (CPC) and (2) a custom made code reproducing, inter alia, the ELPI+ software calculations. The first step is to synchronously save the currents measured by the ELPI+ electrometers and the real total number concentration measured with the CPC. Then, by using the custom-made code for a given measurements interval, an averaged density is adjusted to minimize the gap between the total number concentrations given by the two devices. The NPSD corresponding to this fitted average density is then considered as the closest to the real distribution. This method was validated in laboratory exposure chamber experiments by using a SMPS as a reference for the NPSD. This validation was performed using four UFPs aerosols. In addition to the NPSD, the adequacy of the fitted average effective density with the real size-dependent one was verified. A validation of this method was also successfully performed in electronic waste recycling factories using a Nanoscan SMPS as a reference instead of a SMPS. This method is easy to use in the field or in a laboratory by hygienists or OHS researchers interested by UFPs. Because it allows for the determination of the real average effective density, ELPI+ can be used to collect UFPs particles on its collection substrates for further analysis while recording real-time data of aerosol concentrations that can be rightfully corrected. This method offers also an easy alternative to evaluate particle effective density of any UFP aerosols.

9WA.4

Physical and Chemical Properties of Particulate Matter in a Chinese Electrolytic Zinc Manufacturing Facility. ZIZHEN MA, Xu Huang, Fuyuan Xu, Ge Zhang, Linhua Jiang, Jingkun Jiang, Lei Duan, Ning Duan, *Tsinghua University*

China is the largest producer and consumer of refined zinc in the world. More than 80% refined zinc is produced by hydrometallurgy during which the electrolysis is a key step. During this step, large amount of particulate matter (PM) containing acid mist and heavy metals are generated because of the burst of oxygen bubbles. If not controlled properly, it can lead to significant adverse effects on atmospheric environment and on human health in surrounding area. In this study, PM characteristics in a typical Chinese electrolytic zinc manufacture facility was investigated. TSP, PM_{10} and $PM_{2.5}$ were collected and analyzed for mass concentration and chemical compositions. We found that $PM_{2.5}$ and PM_{10} accounted for 1.6 ~ 3.2% and 29.1 ~ 37.1% of TSP, respectively. TSP contained ~54.0% acid mist in which 47.6% was sulfuric acid and 52.4% was sulfate. The average concentration of acid mist in TSP, PM_{10} and $PM_{2.5}$ was 1.84, 1.54, and 0.11 mg/m^3, respectively. These are higher than the values set by various occupational health and safety regulations in the world. The acid mist collected was unevenly distributed in working place. It increased with the decreasing in the height above the electrolytic bath. Moreover, the acid mist above the electrolytic bath was higher than that those collected in the nearby aisles. The enrichment of acid mist in PM was observed, i.e., the percentage of SO_4^{2-} in PM was more than twice the percentage of SO_4^{2-} in electrolyte. The S_{mol}/Zn_{mol} for $PM_{2.5}$ samples were higher than those in PM10 and TSP samples. Zn, Mg, Mn and Al were the major metallic elements in PM samples. Some hazardous heavy metals (e.g., Pb, Cr, Sb and Cd) were found to be enriched in PM, especially in $PM_{2.5}$.

9WA.5

Exposure of Home Healthcare Workers to Aerosolized Medications: Two-Phase Simulation Study. SERGEY A. GRINSHPUN, Yousef Elmashae, Katie Ollier, Maija Leppänen, Michael Yermakov, Tiina Reponen, *University of Cincinnati*

Home healthcare is one of the most rapidly growing professions worldwide. Home-attending healthcare professionals are exposed to various aerosol contaminants, including pharmaceuticals administered in patients' homes. One common procedure is a nebulizer treatment. Environmental conditions in homes are different from hospital environments, which should affect the aerosol concentration levels and exposure patterns. This two-phase pilot simulation study addressed the inhalation exposure of home healthcare workers to nebulized medications. The objective was to measure particles aerosolized from a commercially available nebulizer-based aerosol delivery system applied to a breathing manikin under different environmental conditions and at different proximity to the aerosol source.

The first phase of this investigation was conducted with aerosolized medications, namely Ipratropium Bromide, Budesonide, and Albuterol Sulfate (all suspended in a NaCl solution), as well as with pure NaCl (also used as medication to treat respiratory symptoms). Deionized water was used as a control. The nebulizer was applied to a manikin connected to a constant push air flow simulating an exhalation-only breathing regime. It maximizes the aerosol output and represents a "worst-case scenario" as compared to a conventional inhalation-exhalation cycle. The other manikin, which simulated a healthcare worker, was placed at different distances from the patient-simulating manikin. The aerosols were measured using an Electrical Low Pressure Impactor (Dekati Ltd). Exposure to all four selected aerosolized medications exceeded background control by one to four orders of magnitude. The particle size distributions measured for the four aerosols at a fixed distance from the source demonstrated similar trends. Although the total aerosol mass concentration in the breathing zone of the healthcare worker-simulating manikin ranged widely, from 0.229 to 1.02 g/m^3, it was not significantly affected by the medication type. We concluded that NaCl can serve as a surrogate for assessing aerosol exposures, at least for the selected nebulizer-administered medications.

The second phase of the study was conducted in a room-size exposure chamber with a breathing manikin simulating a patient. However, instead of applying a constant flow, the manikin was connected to a breathing simulator, producing a cyclic pattern with the mean inspiratory flow rate of 15 L/min. More importantly, instead of using the second manikin representing a healthcare worker, the tests were conducted with an actual human subject whose inhalation point (nose/mouth) located at different distances from the aerosol source: 6", 12", 24", and 48". The total aerosol concentration was measured at these distances using a P-Trak condensation particle counter (TSI Inc.). Based on the findings of the first phase of this study, NaCl was utilized as a medication surrogate. The tests were performed at different air exchange rates in the chamber: 0 (calm air), 5 AEH (a higher end for residential environments), and 17 AEH (extremely high, typically used in stationary healthcare settings). It was concluded that the aerosol concentration (and, therefore, the inhalation exposure) decreases as the worker's proximity to the patient increases. Although statistically significant, this effect was relatively weak: the drop ranged from 1.5- to 2.5-fold when the distance changed from 6" (extremely close proximity) to as far as 48". The air exchange effect was significant between 0 and 5 AEH (typical ventilation rates in homes) with an the average difference of 3-fold; however, it essentially diminished between 5 and 17 AEH.

In summary, the inhalation exposure of home healthcare workers to particles aerosolized by medical nebulizers is significant. The proximity and ventilation affect the exposure; however, these factors are not sufficiently powerful to effectively reduce it.

The study was supported by the National Institute for Occupational Safety and Health through the Targeted Research Training Program of the University of Cincinnati Education and Research Center.

9WA.6

Sources of Particulate Matter in Mines and Mining Environments. Hilkka Timonen, Joel Kuula, Anssi Arffman, Jenni Alanen, Kimmo Teinilä, Matthew Bloss, Minna Aurela, Laura Salo, Risto Hillamo, Sampo Saari, Pedro Oyola, Felipe Reyes, Yeanice Vasquez, Jorma Keskinen, Topi Rönkkö, Eija Asmi, SANNA SAARIKOSKI, *Finnish Meteorological Institute*

Previous studies have indicated, that the main sources of particulate matter in mines are operations associated with mining activities (e.g. drilling, crushing, blasting) and vehicular engine emissions (used in mining machines, ore hauling and for transportation of people) (e.g. Saarikoski et al., 2017). The aim of this study was to conduct detailed characterization of particulate matter (PM) near intensively operating mine. In this study, PM measurements were conducted both at the underground mine and next to open pit mine during spring 2014.

A variety of instruments was used to measure the chemical composition, secondary aerosol formation potential, physical and optical properties of PM near actively operating mining environments. Key instruments of this study include the Soot Particle Aerosol Mass Spectrometer (SP-AMS), the Multiangle absorption photometer (MAAP), aethalometer (AE33), nephelometer (TSI), a scanning mobility particle sizer (SMPS) and potential aerosol mass chamber (PAM). Stationary measurements were conducted at a measurement container located at the maintenance level 500m underground as well as 150m from the open pit mine. In addition, a mobile laboratory, equipped with a large variety of PM instrumentation was used to study spatio-temporal variation of PM in the mine. Low cost sensors were installed to different locations around the mine to test their capability to measure concentrations of fine and coarse particles (PM2.5 and PM10) in the mine in real time.

The concentrations and sources of PM varied in different locations in the mine. Clearly different size distributions and PM compositions for PM were observed at different locations (maintenance level, blasting, crushing, transfer belt and dumping site) at the underground mine. Results of low-cost sensors were comparable to high-end instrumentation results. The benefit of sensors in the mine were easy installation, small size and low cost enabling installation of sensors to several locations simultaneously as a sensor network. In the boreal arctic environment, next to the actively operating open pit mine area, the PM concentrations originating from mining activities were low. Elevated PM and BC concentrations were only observed when wind brought particulate matter from mining area directly to the measurement container. However, when compared to typical urban PM concentrations, the PM concentrations next to the open pit mine were mostly lower.

This project provides important information about the composition of PM and sources in underground and open pit mines as well as novel tools (e.g. sensors) for PM monitoring in mining areas. This information can be used to assess environmental, health and climate impacts of mining in future.

This work was supported by Academy of Finland, (PARMAT, Grant nro 297804), Tekes (HIME project 2-011-2014) and CONICYT, Chile. The great help of the mine staff during the measurement campaigns is highly appreciated.

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9WA.7

Emission and Oxidative Potential of Particulates from Alternating Current Tungsten Inert Gas Welding on Aluminum.

JUN WANG, Shalayne Sims, Jacob Bartels, Marcio Bezerra, *University of Oklahoma*

Welding process generates particulates and gaseous pollutants that are potentially hazardous to welders without adequate ventilation and respiratory protection. Past studies on welding were mainly focused on stainless steel and mild steel with constant feeding direct current (DC). Aluminum (Al) is a common lightweight material that can only be welded with tungsten inert gas (TIG) welding. Al metal plate usually has a tenacious oxide film on the surface that requires being removed through the use of alternating current (AC). AC is achieved through switching between electrode positive and electrode negative polarity at more than 50 cycles per minute. Currently, there is a knowledge gap in understanding the emission of particulates (mostly Al compounds) from Al-AC-TIG welding and their health implications. The scope of this study is to examine whether AC parameters have an effect on the production of particulate Al fume and their oxidative potentials. A conical welding chamber was used to collect metal fumes generated from an AC/DC TIG welder. Welding was performed on a 12×12 aluminum plate and 1/8th inch aluminum filler rods and tungsten electrode, under pure argon shielding gas. The TIG welder's currents vary between 60 and 200 amps. A hurricane high-volume air sampler draws the fume through a 90 mm glass fiber filter. The fume collected on the filter was weighed, and then ultrasonically extracted through water and methanol. The extracts were dried overnight with pure nitrogen flow. The oxidative potentials of extracts were determined using ascorbic acid (AA) assay which showed good sensitivity to transition metal oxides. The rate of AA consumption was calculated using linear regression of the data from a plot of absorbance (265 nm) against concentration gradient/time. The results indicated AC mode can effectively reduce the emission of particulate fume by over 55% comparing to DC mode. Fume emission increased with higher welding currents, with the highest of 335.2 mg/min arc time at 200 A. The consumption of AA showed averaging of 0.2035 nmol of AA/µg of extracts, which is a strong indicator of OP from aluminum oxides. The latter results need to be verified with *in-vitro* cellular reactive oxygen species assays in future studies.

9WA.8

Characterization of Nanometer-Sized Oil Mist Generated in Metal Machining Process. MORIAKI IWASAKI, Kojiro Hirai, Kanta Fukumori, Hidenori Higashi, Takafumi Seto, *Kanazawa University*

Oil mist generated by metal machining has negative effects to human and working environments in the factory. In this study, size distributions of nanometer-sized oil mist generated from three industrial metal (steel) machining process, lathe machining, cutting, and grinding, were investigated using the electrical mobility-based instrument (EEPS, TSI model 3090) and optical particle spectrometer (Welas model 2000) at the exhaust pipe. In all three machining processes, the number concentration of nanoparticles (< 100 nm) increased up to 107 particle/cc after the each machining process started. Peak size of the generated nanoparticles was almost consistent at around 60 nm in the mobility diameter. Condensation of thermally evaporated oil is considered to be major source of nanoparticles in the lathe machining and grinding processes, where water-soluble and insoluble lubricant oil were used, respectively. On the other hand, more steep and clear feature of nucleation and growth was seen in the cutting process, while no lubricant oil was used. In this process, small amount of water-soluble oil remained on the surface of the works after the previous machining process (lathe machining) and these small amount of residual oil might be the precursor of nanoparticles generated in the following cutting process.

In the real industrial processes, the machining was operated in the closed chamber, however, the work pieces were replaced from the front door by the worker. Therefore, the timing for opening the door was synchronized with some time delay from the machining period. In addition, the air of the machining chamber was continuously exhausted in the cutting and grinding process. In spite of these countermeasure, the high number concentration (> 8,000 particles/cc, > 300 nm) of the aerosol was detected at the grinding process, probably because the large consumption of oil (water-insoluble) for cooling the work. It was found that the time delay between opening the door and the exhaust pumping effectively decrease the leakage of oil mist to the working environment of the lathe machining and cutting processes.

10AC.1

Formation and Growth of Aerosol from Agricultural Emissions. PHILIP SILVA, *USDA - Agricultural Research Service*

Particulate matter influences on the environment from agriculture are usually considered to be dominantly coarse mode dust with some secondary component in the fine mode from the impact of ammonia emission. Indeed, some scientists have started investigating whether and how ammonia can interact with anthropogenic and biogenic hydrocarbons to form secondary aerosol. But agricultural emissions include many reactive volatile organic compounds that may potentially contribute to secondary aerosols with or without ammonia. We have performed several field sampling experiments at a poultry house, a dairy, and a hog farm to find evidence for secondary aerosol formation, including new particle formation at the source. We use a scanning mobility particle sizer (SMPS) to acquire size distributions of particles from 10 nm – 0.5 µm in 5-min intervals. Data from the SMPS indicates that particle growth and particle formation events are observed at all facilities by the SMPS very near source. Some formation and growth events are rapid with particle growth exceeding 20 nm per hour. Some data for gas phase measurements of nitrogen- and sulfur-containing compounds will be discussed in terms of whether it is impacting the presence of particle formation or growth events. These data suggest that agricultural emissions may be underestimated as a source for new particulate matter in rural areas and that it is not just the interaction of ammonia with the urban plume that produces secondary aerosol.

10AC.2

Observations of Biogenic New Particle Formation over a Boreal Fen. HEIKKI JUNNINEN, Lauri R. Ahonen, Federico Bianchi, Lauriane Quéléver, Simon Schallhart, Hanna Manninen, Katri Leino, Janne Lampilahti, Stephany Mazon, Jenni Kontkanen, Pavel Alekseychik, Janne Levula, Ivan Mammarella, Timo Vesala, Tuukka Petäjä, Markku Kulmala, *University of Tartu*

Formation of new aerosol particles in the atmosphere is a complicated series of chain reactions, including the production of nanometre-size clusters from precursor vapours, the growth of these clusters to detectable sizes by condensation and the simultaneous removal of clusters by coagulation. It is thought that sulphuric acid is critical in initialization of the particle formation, except in certain coastal regions where iodine oxides are dominating the process. Recent laboratory studies hypothesise that pure organic ion-induced new particle formation could potentially happen also in atmospherically relevant conditions.

In this study, we measured the composition of biogenic volatile organic compounds (BVOC) emissions from a wetland, depletion of O3 and formation of the oxidation products of emitted BVOCs. We also show the involvement of produced low volatile organic compounds in atmospheric new particle formation.

The measurement campaign was conducted in a boreal wetland close to the Station for Measuring Ecosystem-Atmosphere Relations II (SMEAR II). The vegetation of the site is dominated by different sedges and a continuous Sphagnum carpet. The fen acts as a source of methane throughout the year with the maximum during the summer time and minimum during the coldest season. The CO_2 fluxes in contrary have a negative annual balance -156 g m^{-2}, equals -42.5 g-C m^{-2}.

The site is equipped with permanent measurements for basic meteorology and for CO_2, H_2O, and CH_4 fluxes. Additionally, the chemical composition of atmospheric ions was measured with atmospheric pressure interface time-of-flight mass spectrometer (APi-TOF), concentrations of sulfuric acid (SA) and low volatile oxygenated organics (highly oxidized multifunctional molecules, HOM) with chemical ionization with nitrate chemistry (NO_3-CI)-APi-TOF. Volatile organic compounds (VOC) were measured with proton transfer reaction (PTR)-TOF. Atmospheric cluster and aerosol size distribution was measured with Neutral clusters and Air Ion Spectrometer (NAIS) and nano-particles.

During the campaign, we observed several new particle formation events. The events observed during the day time (NPFd) had the same characteristics as the ones observed in forest station, 10 km away. During NPFd the sulphuric acid was the one single most increasing component. However, during the night time events (NPFn) the observed chemistry was considerably different. The most prominent difference was the decrease of O_3 concentration to as low levels as 2-5 ppb. At the same time the concentrations of nitrogen containing HOMs increased by an order of magnitude, but non-nitrogen containing HOMs decreased. This behaviour points towards a purely organic oxidation and formation of new particulates, without involvement of SA.

These events became more frequent after the snow melt and the increased temperature difference between day and night. Low relative humidity and low wind speeds are also associated with the observed night time organic new particle formation events.

In the presentation observed organic oxidation and consecutive new particle formation will be discussed in details.

This work is supported by the Academy of Finland Centre of Excellence (grant no. 272041), the European Union’s Horizon 2020 research and innovation program (grant No 654109), European Research Council (ERC-StG COALA), European Regional Development Fund and Estonian Research Council programme Mobilitas Pluss project MOBTT42 and we thank the tofTools team for providing tools for mass spectrometry analysis.

10AC.4

The Impact of Multiphase Chemistry on Nanoparticle Growth and Composition. MICHAEL J. APSOKARDU, Murray Johnston, *University of Delaware*

Carbonaceous matter is responsible for a substantial fraction of the growth of nanoparticles in the atmosphere to a climatically relevant size. Highly oxidized organic molecules (HOMs) formed in the gas phase by oxidation of a precursor molecule will grow pre-existing particles when they partition to the particle phase. Non-volatile molecules grow particles at the condensation rate since re-evaporation is negligible. Semi-volatile molecules grow particles at a rate slower than the condensation rate since re-evaporation is significant. Chemical reactions in the particle phase that convert semi-volatile reactants into non-volatile products can increase the growth rate because additional semi-volatile molecules must flow from the gas phase to the particle phase in order to replace the molecules lost through reaction. This combination of gas-particle partitioning with subsequent reaction in the particle phase is termed multiphase chemistry. The impact of multiphase chemistry on particle growth depends on the mixing ratios and volatility distributions of HOMs in combination with their particle phase reaction rates. We have developed a kinetic model for nanoparticle growth that is able to explore these factors, and we have used it to interpret several types of experiments in flow tube reactors. For example, we find that the large fractions of oligomeric species detected by ESI-HRMS in SOA originating from OH oxidation of decamethylcyclopentasiloxane (D5) and ozone oxidation of monoterpenes require particle phase reaction rate constants in the 10^{-3} to 10^{-1} $M^{-1}s^{-1}$ range. Rate constants of this magnitude are consistent with those measured for reactions of hydroperoxides and/or peroxyacids with carbonyls to form oligomers. Most recently, we have compared experimentally measured growth rates of monodisperse seed particles to those predicted from model calculations. Calculations based on condensation of non-volatile HOMs produced in the flow tube reactor are generally able to reproduce the experimental results, though they have a tendency to under predict growth rates in some cases, suggesting that multiphase chemistry can contribute to particle growth. By systematically comparing experimental measurements with model calculations, we are able to predict the situations where multiphase chemistry is most likely to enhance nanoparticle growth in the atmosphere.

10AC.5

Formation of Secondary Aerosol and Growth of New Particles in the Ambient Atmosphere: An Experimental Study Using a Dual Smog Chamber System.

SPIRO JORGA, Christos Kaltsonoudis, Spyros Pandis, *Carnegie Mellon University*

Laboratory or field smog chamber experiments using as a starting point ambient air can improve our understanding of the evolution of atmospheric pollutants at timescales longer than those achieved by traditional laboratory experiments. Use of two identical smog chambers, with the first playing the role of the baseline chamber and the second the perturbation chamber (e.g. addition of oxidants) can assist in the interpretation of the results in such inherently complex chemical systems. The differences of the measurements in the two chambers can be used as the basis for the study of the corresponding chemical or physical processes.

In this work a set of two identical Teflon pillow-shaped smog chambers (1.5 m^3 each) are used to study the production of secondary organic aerosol (SOA) and the evolution of the preexisting OA in an urban area (Pittsburgh, US). The two chambers are surrounded by UV lamps. The perturbation induced in one of the chambers is the addition of hydroxyl radicals (OH) formed from the photo-dissociation of HONO or H_2O_2. The aerosol composition in both chambers was continuously characterized using an aerosol mass spectrometer, while the concentration of organic gases using a proton transfer reaction mass spectrometer. Nucleation and growth of new particles was observed in the perturbation chamber in several experiments. At the same time, significant secondary organic aerosol production was observed much higher than what is expected from the oxidation of the present volatile organic compounds. The results of a series of experiments are analyzed to evaluate our understanding of the processing of this complex aerosol and its precursors under these controlled conditions. The implications for SOA and new particle formation are discussed.

10AC.6

Investigation of New Particle Formation from Aromatic Hydrocarbons: Impact of OH and NOx on Highly Oxidized Multifunctional Compounds. HOUSSNI LAMKADDAM, Mao Xiao, Christopher R. Hoyle, Lubna Dada, Mingyi Wang, Dominik Stolzenburg, Lukas Fischer, Andrea Baccarini, Chuan Ping Lee, Ruby Marten, Imad El Haddad, Josef Dommen, Urs Baltensperger, CLOUD Collaboration, *Paul Scherrer Institute*

Aerosol particles in the atmosphere are ubiquitous. Despite their tiny size, aerosols exert an important impact on human health, clouds and global climate. Understanding new particle formation (NPF) is an essential step since nucleated particles might contribute to 50% of the cloud condensation nuclei (CCN) (Merikanto et al. 2009; Dunne et al. 2016).

Our current knowledge of the physical and chemical mechanisms controlling NPF is still poorly constrained. This lack of a robust framework on NPF processes results in a large uncertainty of model outputs – i.e. long-term prediction of CCN – and hence past and future change in climate.

Recently, laboratory and field campaigns have shown evidence for NPF from highly oxidized multifunctional compounds (HOMs) in the absence of sulfuric acid (H2SO4) while that molecule was thought to be absolutely required (Kirkby et al. 2016; Bianchi et al. 2016). However, studies highlighting the role of HOMs in the aerosols growth and NPF were predominantly performed on anthropogenic-free activities, i.e. experiments carried out with biogenic precursors and without NOx (Riccobono et al. 2014; Kirkby et al. 2016; Frege et al. 2018). Therefore the representation of NPF in urban environment is an area of research where data are urgently needed.

In this context, the aim of this work is to study NPF from aromatic hydrocarbons (ArHCs) which represents a dominant source of emitted volatile organic compounds in urban areas. The project aims also at building a NPF database by providing a parameterization which represents the physical and chemical processes (NOx, NH3, H2SO4…) leading to NPF in air quality model.

The CERN CLOUD (Cosmic Leaving Outdoor Droplets) chamber was used to study the HOMs production from individual and mixtures of ArHCs under atmospherically relevant concentration of NOx, NH3 and H2SO4. Selected ArHCs are toluene, 1,2,4-trimethylbenzene and naphthalene.

We will present to which extent the HOMs production yields and particle formation rates are impacted by NOx and OH level for each precursor and their respective mixture.

The research is supported by the Swiss National Science Foundation and the MSCA-ITN project CLOUD-MOTION no. 764991. We thank CERN for supporting CLOUD with important technical and financial resources, and for providing a particle beam from the Proton Synchrotron. We acknowledge tofTools software for mass spectrometry analysis.

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10AC.7

Recent Advances in Understanding on the Relation between Ion Composition and Ion-induced Nucleation in the Boreal Forest in Southern Finland. CHAO YAN, Clemence Rose, Lubna Dada, Federico Bianchi, Siegfried Schobesberger, Heikki Junninen, Katrianne Lehtipalo, Wei Nie, Tuija Jokinen, Nina Sarnela, Yonghong Wang, Qiaozhi Zha, Olga Garmash, Mikko Sipilä, Tuukka Petäjä, Veli-Matti Kerminen, Mikael Ehn, Markku Kulmala, *University of Helsinki, Finland*

New particle formation (NPF) potentially contributes to a significant fraction of the atmospheric aerosol particles, hence affect the air quality and climate. One critical step of NPF is to form stable clusters for sebsequent condensational growth. Recent chamber studies have demonstrated the significant enhancement of NPF by atmospheric ions stabilizing the initial clusters (the so-called ion-induced nucleation, e.g., Kirkby et al., 2011, Kirkby et al., 2016). However, it has remained unclear if these chamber findings are directly applicable to the more complicated atmosphere, mostly due to the incomplete understanding of the formation of atmospheric ion clusters as well as difficulties in characterizing their subsequent growth.

The ion composition has been first measured by Ehn et al., (2010) at the boreal forest in southern Finland (Hyytiälä station) using an atmospheric-pressure-interface time-of-flight mass spectrometer (APi-TOF). The results revealed clear diurnal variation of the ion composition: Sulfuric acid ion clusters are dominant during the daytime, whereas adducts of highly oxygenated organic compounds (HOM) and nitrate (HOMNO3-) are more prominent during the night. This observation has recently been deepened by Bianchi et al., (2017), who have categorized ion cluster composition into finer groups: Clusters of nitrate- or non-nitrate HOMs with HSO4- or NO3- adducts were explicitly separated. However, it has not been dedicatedly studied how ion composition affects IIN.

We characterized the anion composition and IIN at the Hyytiälä station using longer data sets from 3 consecutive springs (2011-2013, 167 measurement days in total), with a special focus on the relation between ion composition and IIN. Our results show that IIN at Hyytiälä station is driven by different mechanisms, which vary diurnally and seasonally. More specifically, H2SO4-NH3 and HOM clusters drive daytime IIN alternately, which is regulated by temperature, whereas all nighttime IIN events are driven by HOM clusters. The observational details of the formation and growth of ion clusters will be presented.

10AC.8

SALTENA Campaign: A Comprehensive Study of New Particle Formation (NPF) at Mt. Chacaltaya (5240m A.S.L.) in South America. QIAOZHI ZHA, Diego Aliaga, Otso Peräkyla, Yee Jun Tham, Xuemeng Chen, Joonas Enroth, Liine Heikkinen, Katrianne Lehtipalo, Juha Kangasluoma, Mikael Ehn, Mikko Sipilä, Tuukka Petäjä, Markku Kulmala, Claudia Mohr, Federico Bianchi, *University of Helsinki*

Atmospheric aerosol particles play an important role in the Earth's radiation balance, and have a strong effect on climate. A significant contributor to atmospheric aerosol loading is new particle formation (NPF), which can produce up to 50% of the world's cloud condensation nuclei (CCN). While fruitful results from field measurements have been reported over past decades, only a handful of studies have been conducted at high altitudes, where NPF events are frequently observed. Recent studies from Jungfraujoch station (3580m a.s.l.) in Central Europe reveal that NPF in the free troposphere was majorly driven by the condensation of highly oxygenated molecules (HOMs). However, the exact mechanism of free-tropospheric NPF in the Southern Hemisphere has remained unclear.

The ongoing Southern hemisphere high ALTitude Experiment on particle NucleAtion and growth (SALTENA) campaign started in December 2017, and is expected to finish in June 2018 in the Chacaltaya station (5240m, a.s.l.) in Bolivia. The station is approximately 30km away from city area of La Paz. A set of state-of-the-art instruments were deployed to systematically study the previously reported frequent NPF events. Information on the chemical composition of ion clusters was provided by an Atmospheric Pressure interface Time-Of-Flight mass spectrometer (APi-TOF). Atmospheric HOMs and sulfuric acid (SA) concentration were measured with a nitrate ion based Chemical Ionization APi-TOF (CI-APi-TOF). Aerosol chemical composition was measured with an Aerosol Chemical Speciation Monitor (ACSM). The concentration and size distribution of aerosol particles were measured with a particle size magnifier (PSM), a neutral cluster and air ion spectrometer (NAIS, also measuring ion cluster concentrations), and a scanning mobility particle sizer (SMPS). Trace gases, solar radiation, and meteorological parameters were also monitored.

Preliminary results from SALTENA show that NPF events are usually observed with the air masses originating from the city area, the air contained high SA concentrations and large amount of sulfuric acid-ammonia (SA+NH3) clusters, suggesting SA+NH3 nucleation might play an important role in such an environment. Nucleation could be also observed when air masses came from Amazon area, which involved abundant HOM molecules. In this presentation, a more detailed chemical analysis of the high altitude NPF events will be presented.

10AC.9

Temperature and UV Light Affect HOM Chemistry and Biogenic New Particle Formation. MARIO SIMON, Lubna Dada, Martin Heinritzi, Lukas Fischer, Dominik Stolzenburg, Xucheng He, Chao Yan, Andrea C. Wagner, Andreas Kürten, Jasper Kirkby, Joachim Curtius, *Goethe University Frankfurt*

New particle formation (NPF) is an important source of global aerosol loadings and has been reported under a variety of conditions ranging from marine, remote or urban areas, as well as at ground level, free and upper troposphere. Recently it has been shown that the highly oxygenated molecules (HOMs) formed by the oxidation of monoterpenes ($C_{10}H_{16}$) contribute to NPF and are even able to form particles at atmospherically relevant concentrations without further assistance of other low volatile compounds (e.g sulfuric acid) (Kirkby et al., 2016; Tröstl et al., 2016).

These HOMs form mostly via an initial oxidant (e.g. O_3, OH or NO_3) attack on the double bound of the monoterpene, which leads to peroxy radicals (RO_2). The highly reactive RO_2 radicals undergo rapid autoxidation steps due to subsequent intramolecular H-shifts and form progressively higher oxygenated RO_2 radicals (Crounse et al., 2013). The termination products of these reactions are highly oxygenated monomers and even covalently bound dimers which are thought to be responsible for nucleation due to their extremely low volatility (Ehn et al., 2014). The oxidation pathway of HOMs are very sensitive to different environmental conditions and therefore resulting in strong variation of pure organic NPF and a large uncertainty in global aerosol models.

In this study, we show data from the Cosmics Leaving OUtdoor Droplets (CLOUD) experiment at CERN to investigate HOMs formation from the most abundant monoterpene α-pinene and NPF under a large variety of conditions. A nitrate based chemical ionization atmospheric pressure interface Time-of-Flight mass spectrometer (CI-API-TOF) was used to measure neutral HOMs and characterize their chemical composition. Furthermore, a newly developed proton transfer reaction mass spectrometer (PTR-MS) instrument was used to quantify also the low to semi-volatile organic compounds (LVOC and SVOC) to understand their interactions and to complete the picture of their chemistry and formation rate. The nucleation rates of these comprehensive experiments were determined using several particle counters including Particle Size Magnifiers (PSM), Condensation Particle Counter (CPC) as well as a nano-Scanning Mobility Particle Sizer (nanoSMPS).

We studied the effect of temperature on HOM chemistry and NPF at four different temperatures (-50, -25, +5 and +25°C) and various concentrations to simulate a wide range of atmospheric latitudes and altitudes where NPF can occur. Therefore, we measured the impact to the autoxidation rate as well as the RO_2 radical termination and the closed shell product distribution of HOMs. Additionally, we investigated the effect of UV light on the HOM chemistry. Furthermore, we discuss the question in how far the formation rate of new particles is affected by temperature and UV changes.

Our results improve the understanding of pure biogenic nucleation as we extend the range of conditions studied. This knowledge also helps to improve the predictions of global aerosol models for very clean environments as well as the pristine pre-industrial climate.

10AC.10

Investigation of Multicomponent New Particle Formation under Urban Atmospheric Conditions in the CLOUD Chamber. MAO XIAO, Christopher R. Hoyle, Lubna Dada, Mingyi Wang, Dominik Stolzenburg, Lukas Fischer, Andrea Baccarini, Chuan Ping Lee, Houssni Lamkaddam, Ruby Marten, Imad El Haddad, Josef Dommen, Urs Baltensperger, CLOUD Collaboration, *Paul Scherrer Institute*

The formation of new particles from atmospheric vapors (new particle formation, NPF) is an important atmospheric process having great effects on the particle number concentration and size distributions. Urban atmospheres are highly polluted with high concentrations of sulfuric acid, ammonia, NOx and volatile organic gases primarily emitted from anthropogenic activities. Despite the high particle concentrations in polluted air, which are unfavorable for NPF, NPF is still reported to occur with high frequency and at high formation rates in highly-polluted urban environments.

Photochemical air pollution in the urban atmosphere is often dominated by anthropogenic volatile organic compounds, containing a high fraction of aromatic hydrocarbons originating from industrial activities, traffic and residential wood combustion. Observations of highly oxygenated molecules forming in OH-triggered oxidation of aromatic hydrocarbons (Molteni *et al.*, 2018; Wang *et al.*, 2017) suggest that aromatics could be potential precursors for NPF especially in the polluted atmosphere. Another potential class of compounds participating in NPF in a polluted atmosphere is amines. Amines in urban air may enable high formation rates under atmospherically relevant sulfuric acid concentrations. Amine enhancement of NPF is known from earlier chamber studies (Almeida *et al.*, 2013), but this effect was believed to be only significant when it is close to the amine sources due to the short life-times of gaseous amines.

To investigate the role of amines and aromatic hydrocarbons in NPF under polluted urban atmospheric conditions, experiments were conducted at the “Cosmics Leaving OUtdoor Droplets” (CLOUD) facility at the European Organization for Nuclear Research (CERN). New particle formation from the mixtures of naphthalene, 1,2,4- trimethylbenzene and toluene, sulfuric acid and ammonia in the presence of NOx were studied with and without the addition of 0.4 ppt dimethylamine at 278 K and 293 K. New particle formation rates and early growth rates calculated for each temperature. New particle formation rates and early growth rates derived for each temperature as well as the enhancement with the addition of dimethylamine will be reported. Low temperature favors NPF both with and without dimethylamine addition. The contribution of sulfuric acid, nitric acid and organics to sub-3 nm particle growth is also evaluated based on particle composition measurements.

The research is supported by the Swiss National Science Foundation and the MSCA-ITN project CLOUD-MOTION no. 764991. We thank CERN for supporting CLOUD with important technical and financial resources, and for providing a particle beam from the Proton Synchrotron. We acknowledge tofTools software for mass spectrometry analysis.

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10AC.11

Interactions between Aerosol Compositions and Liquid Water Content during Beijing's Haze Episodes at Different Seasons. XIAOXIAO LI, Wei Zhou, Jiming Hao, Jingkun Jiang, *Tsinghua University*

Aerosol liquid water (ALW) is an abundant composition in atmospheric aerosol. It is believed to play an important role in both secondary organic and inorganic formation through elevating gas-particle transformation, heterogeneous and aqueous reactions, especially in region with high RH. To explore the interactions between ALW and aerosol compositions during haze formation and evolution in Beijing. ALW were modeled based on long term measurement of non-refractory submicron aerosol compositions in different seasons in Beijing. The water content contributed by inorganics was modelled by ISORROPIA version 2.0 using both thermodynamic and metastable mode. The water content contributed by organics was estimated using the Zdanovskii-Stokes-Robinson(ZSR) mixing rule with κ-Köhler theory. In which κ is a real-time variation value related to the real time O: C ratio of organics instead of using a fixed value of 0.1 often used in previous calculations. Organic water in Beijing accounts for 7-33% of total water, the highest proportion happens in the cleanest days when the proportion and oxidation state of organics are both higher. During haze evolution, although the fraction of organics decreases with an increase in aerosol mass loading, the proportion of water content contributed by organics to the total aerosol mass is still increasing. The influence of water to aerosol compositions was explored by looking at the variation of acid/base, SO_4^{2-}/NO_3^- and O/C during haze episodes which behave totally different with high and low ALW. In low-ALW episodes acid/base, SO_4^{2-}/NO_3^- and O/C do not change much with haze evolution and O/C even decreases at high volatile species partitioning. While during high-ALW episode, acid/base, SO_4^{2-}/NO_3^- and O/C increase with haze evolution. The increasing O/C ratio indicates the formation of more soluble organics, such as carboxylic acid which will increase the hygroscopicity and thus further increase water uptake. Most of the 23 classified haze episodes are high-ALW episodes. A few previous studies proposed a positive feedback loop that an increase in RH leads to an increasing aerosol inorganic fraction and subsequently increase the rate of water uptake. This study indicates that this loop also exists for aerosol organic species in Beijing.

10AC.12

Laboratory Investigations of SOA Photolysis. MARIA ZAWADOWICZ, John Shilling, *Pacific Northwest National Lab*

Secondary organic aerosol (SOA) accounts for a large fraction of tropospheric particulate matter in accumulation mode. Accurate representation of SOA life cycle in models is needed to quantify its effects on radiative forcing and air quality. While SOA production rates and mechanisms have been extensively investigated, the exact loss pathways are still uncertain. Most current large-scale models account for dry and wet removal of SOA, but not for chemical losses, such as photolysis or surface oxidation by OH and ozone. Model estimates indicate that introducing an SOA photolysis rate equivalent to 0.04% of typical NO_2 photolysis rate can lower tropospheric SOA mass by 40 – 60%. Laboratory measurements of SOA photolysis rates are necessary to better constrain theoretical estimates. This study reports a series of batch-mode environmental chamber experiments quantifying UV photolysis rates of atmospherically-relevant SOA types. These experiments aim at assessing the photolytic contribution to SOA removal for several precursors (including isoprene, α-pinene and toluene), high- and low-NO_x pathways and different RH conditions.

10AC.13

Explaining Atmospheric Particle Growth by Organic Vapors of Biogenic and Anthropogenic Origin. CLAUDIA MOHR, Taina Yli-Juuti, Joel A. Thornton, Felipe Lopez-Hilfiker, Anna Lutz, Arto Heitto, Juan Hong, Neil Donahue, Ilona Riipinen, Wei Huang, Cheng Wu, Federico Bianchi, Qiaozhi Zha, Diego Aliaga, Liine Heikkinen, Markku Kulmala, Marcos Andrade, *Stockholm University*

The ability of atmospheric aerosols to act as cloud condensation nuclei (CCN) is influenced by both the particles´ size and chemistry. For particles formed in the atmosphere via nucleation of vapors, this means that they must undergo significant growth before they can become active as CCN. The identification of the condensable organic vapors driving particle growth, and their sources, is thus fundamental for simulating changes to aerosol-cloud interactions, which are one of the most uncertain aspects of anthropogenic climate forcing.

We present particle growth studies from a combination of ambient measurements and process modelling at two locations influenced by new particle formation. We used measured concentrations of oxygenated organic vapors in ambient air as input for the particle growth model MABNAG to investigate identity and nature of the condensable organic vapors driving growth of newly formed particles.

Gas phase concentrations of oxidized organic species were measured in the boreal forest at Hyytiälä, Finland, in spring 2014 with a chemical ionization high-resolution time-of-flight mass spectrometer with a filter inlet for gases and aerosols (FIGAERO-CIMS), using iodide as reagent ion. Based on derived molecular formulae of the measured compounds, we calculated their saturation concentrations, and grouped them in a 1-D volatility basis set (VBS). The time series of the organic concentrations grouped in the VBS, together with measured gas concentrations of sulfuric acid and ammonia, relative humidity and temperature, were then used to model the change in size and composition of a newly formed particle under the given ambient conditions. Simulated particle growth rates matched the observed particle growth rates measured with a differential mobility particle sizer within uncertainties. These results suggest that the measured distribution of gaseous oxygenated organic compounds is sufficient to explain particle growth to CCN-active sizes at this location. Most of the simulated growth can be assigned to condensation of low- or extremely low-volatile organic compounds, with significant contributions from nitrate containing compounds. A comparison of measured and modelled evaporative behavior of the grown particles indicates a negligible contribution of particle phase reactions, and points to gas-phase reactions and subsequent condensation of reaction products to be the main driver for particle growth under these conditions.

We also present particle growth observations from a distinctively different environment, where direct atmospheric observations of the life cycle and chemistry of aerosol particles from nucleation to cloud droplets are still scarce. We show first results from a comprehensive 6-month field campaign (December 2017 – May 2018) conducted at the GAW station Chacaltaya in the Bolivian Andes, at 5240 m a. s. l. The influence of the emissions from the nearby city of La Paz, and of air masses from the Amazon during the rainy season, make this a highly interesting site to study atmospheric particle formation and growth processes. To this purpose we deploy several state-of-the-art mass spectrometers. For this presentation we focus on results from the FIGAERO-CIMS and investigate the nature and relative importance of anthropogenic and biogenic organic components contributing to particle growth.

10AC.14

Impact of Ammonia on Atmospheric (H2SO4)n(HSO4-) Ions: Thermochemistry and Implications for New Particle Formation. ALEXEY NADYKTO, Jason Herb, Kirill Nazarenko, Fangqun Yu, *Moscow State University of Technology; SUNY at Albany*

Ion-Mediated Nucleation (IMN), which involves, in addition to H_2SO_4 and H_2O, common airborne ions and other stabilizing species, is an essential source of secondary particles [1-3]. Typically, airborne ions have great advantage over neutrals with regards to uptake of highly dipolar ($\mu(H_2SO_4)$ = 3.02 D; $\mu(H_2O)$=1.85 D; $\mu(NH_3)$=1.44 D) monomers of atmospheric nucleation precursors and multicomponent neutral clusters. However, bonding of NH_3, the most abundant atmospheric base, to common atmospheric ion HSO_4^- exhibits non-classical behavior. In particular, charged $(HSO_4^-)(NH_3)$ complex appears to be much less stable thermodynamically than its neutral analog ammonium bisulfate $(H_2SO4)(NH_3)$, exhibiting a perfect example of inability of the Classical Nucleation Theory (CNT) to adequately describe nucleation thermochemistry . Nonetheless, larger stable $(H_2SO_4)_n(HSO_4^-)(NH_3)_m$ clusters have been observed in laboratory experiments under atmospherically relevant conditions. However, both the molecular nature of the stabilizing effect of NH_3 on $(H_2SO_4)_n(HSO_4\text{-})(NH_3)_m$ formation mechanism remain puzzling.

The main goals of this paper is to gain new insights of the stabilizing effect of NH_3 on $(H_2SO_4)_n(HSO_4^-)$ clusters and to elucidate the $(H_2SO_4)_n(HSO_4^-)(NH_3)_m$ formation mechanism. In order to achieve the goals, we have carried a DFT study at PW91PW91/6-311++G(3df,3pd) level, have examined structural trends, have obtained and analyzed new thermochemical data. We have also investigated dependencies of cluster formation energies on *n* and *m*, explored cluster distributions under atmospherically relevant conditions and discussed implications of new data for interpreting nucleation experiments and observations of NPF and constraining nucleation models.

The present study leads us to conclude that

(1) Ammonia affects both average S-S and N-S distances in $(H_2SO_4)_n(HSO_4^-)(NH_3)_m$. While NH_3 effect is size- and composition- dependent, at n>2, addition of any number of NH_3 molecules to pure negatively charged $(H_2SO_4)_n(HSO_4^-)$ leads to the reduction in the average S-S distances that in turn indicates the enhanced overall stability of larger $(H_2SO_4)_n(HSO_4^-)(NH_3)_m$ clusters.

(2) The strength of the interaction of $(H_2SO_4)_n(HSO_4^-)(NH_3)_m$ clusters with H_2SO_4 , the key atmospheric nucleation precursor, increases as the molar fraction of NH_3 is growing. This indicates that the presence of NH_3 enhances the stability of nucleating $(H_2SO_4)_n(HSO_4^-)(NH_3)_m$ ions.

(3) Although small negative ions are known to be unstable under typical atmospheric conditions, the analysis of the thermochemical data obtained in the present study confirms that NH_3 can get into and stabilize larger (n>2) negatively charged ions. This seems to explain the presence of ammonia in large stable $(H_2SO_4)_n(HSO_4^-)$ clusters and a pronounced effect of NH_3 on stability of large negatively charged H_2SO_4 cluster ions observed in laboratory experiments despite the extreme instability of the ammonium bisulfate ion.

(4) The comparison of distributions of $(H_2SO_4)_n(HSO_4^-)(NH_3)_m$ clusters shows that at n=3 and n=4 most abundant ions under typical atmospheric conditions contain, in agreement with observations, at least one and two NH_3 molecules, respectively.

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10AC.15

Effects of Temperature on Nucleated Particles from α-Pinene Ozonolysis Measured by a FIGAERO-Chemical Ionization Mass Spectrometer. QING YE, Mingyi Wang, Victoria Hofbauer, Dexian Chen, Jasper Kirkby, Neil Donahue, CLOUD Collaboration, *Carnegie Mellon University*

Oxidation products from α-pinene ozonolysis form particles that will scatter sunlight and nucleate clouds. These products, formed via various reaction pathways under different environmental conditions, have a wide range of volatilities and structures that will determine both their gas-particle phase partitioning and their tendency to participate in condensed phase reactions. It has been shown that highly oxygenated multifunctional molecules (HOMs) from α-pinene ozonolysis contribute to nucleation and particle initial growth. Thus understanding the formation of HOMs is crucial to constrain particle loading in the pre-industrial atmosphere. Recent research shows that HOMs are formed via autooxidation process where highly oxygenated RO_2 radicals are formed through multiple cycles of intramolecular hydrogen abstraction and O_2 addition to the initial RO_2 radicals from α-pinene ozonolysis. The autooxidation process, which is a unimolecular reaction, is strongly temperature dependent, and low temperature slows down the autooxidation rate. Therefore, nucleation and initial particle growth is expected to reduce. On the other hand, low temperature favors condensation of materials with higher volatilities (semi-volatiles become low-volatiles and low-volatiles become extremely low-volatiles at low temperature), which are presumably less polar and oxygenated. Thus, composition and properties of the nucleated particles at different temperatures could be very different.

Chemical ionization mass spectrometry coupled with a filter inlet for gas and aerosols (FIGAERO-LToF-CIMS) can measure the chemical composition of gas and condensed phase products from α-pinene ozonolysis with high time resolution and high mass resolution. We deployed a FIGAERO-LToF-CIMS with iodide as the reagent ion in the experiments in the Cosmics Leaving Outdoor Droplets (CLOUD) chamber at CERN. In the experiments, particles were formed through pure organic nucleation under 3 different temperatures, 25°C, 5°C and -50°C with 600 ppt α-pinene and 40 ppb ozone without the addition of NO_x and under dark conditions. When gas phase products were analyzed by the CIMS, particle phase products were being collected on the Teflon filter for 30 mins. During the particle measurement mode, the filter was heated up to 170°C from room temperature to evaporate materials collected on the filter and the materials were then analyzed by the mass spectrometer.

Our preliminary results show that we are able to clearly measure the monomers (C8−10 compounds) and dimers (C16−20 compounds) in the particle phase under all temperatures in our experiments. At 5°C, both the monomers and dimers mass range contain products with higher oxygen number than at -50°C, and the overall O/C is higher at 5°C than at -50°C. At 25°C, oxidized products in the particles contain molecules with 6 oxygens or more while at -50°C, molecules with 3 oxygens start to appear in the particles phase. In addition, we observed more fragmentation (increased fraction of C8−9 compounds in monomers and increased fraction of C16−19 compounds in dimers) at higher temperature than at low temperature. Our work will provide better understanding on particle formation and properties of the nucleated particles from α-pinene ozonolysis at different atmospheric temperature conditions.

10AC.16
Tracking Carbon during the Formation of Secondary Organic Aerosol from Alkane Oxidation. JOSHUA MOSS, Abigail Koss, Jesse Kroll, *MIT*

Secondary organic aerosol (SOA) comprises a major fraction of particulate matter in the atmosphere and is principally formed via the oxidation of volatile organic compounds (VOCs). This study is primarily focused on understanding SOA formation and evolution from alkanes, likely to be key contributors to particulate matter in urban environments. In general, laboratory chamber studies aimed at elucidating the underlying chemical mechanisms pertaining to SOA formation and evolution have been unable to enumerate all organic species produced in SOA-forming reactions, largely due to the extreme chemical complexity of the system. Alkane chamber studies are challenging also because their relatively slow oxidation rates make it difficult to understand later-generation aging chemistry. Additionally, understanding SOA yields and formation mechanisms from chamber studies can be challenging due to poorly-constrained depositional losses of vapors to chamber walls. Despite substantial study in recent years, these remain uncertain and difficult to predict, varying from species to species and even from chamber to chamber. Such vapor losses may also decrease SOA yields in chamber studies and could contribute to differences in the chemistry observed in chambers from that observed in the atmosphere. Here we describe the results of a series of chamber experiments designed to probe the underlying mechanisms related to alkane SOA formation and evolution. We employ a suite of analytical instruments to perform detailed chemical analysis of alkane oxidation products in conjunction with a technique to measure Total Suspended Carbon (TSC) enabling the direct quantification of wall losses and providing a new constraint on the extent of “carbon balance” measured in atmospheric oxidation studies. These chamber photo-oxidation experiments provide a mechanistic understanding of alkane SOA aging, as well as insights to the role of wall losses of various oxidation products. Additionally, we make direct comparisons between the “bottom-up” measurements obtained from the suite of gas- and particle-phase instruments and the “top-down” constraint imposed by the TSC instrument to understand how wall losses affect SOA formation and aging in chambers.

10AC.17

The Role of Iodine Emission in the Atmospheric Aerosol Formation. RAVI KUMAR, *Multanimal Modi College, Modinagar-201204 (U.P.), India*

Recent studies have shown that new particle formation via a secondary gas-to-particle process at coastal regions (see review articles of Kolb, 2002 and von Glasow, 2005) originates from biogenic emissions (Carpenter, 2003) of iodine-containing vapours such as CH_2I_2 and I_2. These species undergo rapid photo-chemical reactions to produce condensable iodine oxides which, in turn lead to the nucleation and growth of new particles (O'Dowd and Hoffmann, 2005).

These particles may be ubiquitous in the Earth's atmosphere if open ocean sources are also significant. They may influence the global radiation budget directly i.e. they can scatter and absorb solar radiation to some extent and may therefore affect climate. In terms of an indirect effect, a significant fraction of these particles have the potential to grow into cloud condensation nuclei (CCN). Changes in the number concentration of CCN may affect the number concentration and size of cloud droplets, and therefore the optical properties and the lifetime of clouds (Curtius, 2006).

Despite the recent studies, uncertainty still remains regarding the composition of newly formed particles from photo-oxidation of iodine-containing species. According to Saunders & Plane (2005), the most likely composition of particles is I_2O_5 while studies of particle formation from photolysis of CH_2I_2 (Jimenez et al., 2002; O'Dowd and Hoffmann, 2005) have suggested the I_2O_4 form. However, a thorough knowledge of atmospheric particle composition and properties requires a description of how they interact with other gases (H_2O and H_2SO_4 in particular) in the marine boundary layer (MBL).

This study will report laboratory studies, including: the formation and growth kinetics of iodine oxide nano-particles, and their uptake of water and sulphuric acid; the redox kinetics of iodate/iodide ions in aerosols; and the action of O_3 in releasing I_2 from aqueous iodide.

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10AP.1

Photopolarimetric Light Scattering to Place Constraints on Dust Properties. GORDEN VIDEEN, Evgenij Zubko, *US Army Research Lab*

Light scattering is a function of particle composition and morphology. The goal of remote sensing is to gain such information about these particles from their scattered light, the so-called inverse problem. It has long been recognized that an exact solution to this problem cannot be achieved. However, recent advances have allowed us to place constraints on the system, that when combined with a priori knowledge, can provide significant information. A number of successes have been realized in the field of planetary science.

10AP.2

Dependence of Heterogeneous Nucleation of N-Butanol Vapor on Temperature and Humidity for improved detection of Nanoparticles. CHRISTIAN TAUBER, Gerhard Steiner, Paul M. Winkler, *University of Vienna*

Commercial Condensation Particle Counters (CPCs) are mainly used to measure the number concentration of airborne particles (McMurry, P. H. (2000). Atmospheric Environment, 34(12-14):1959-1999). Most ultrafine continuous flow CPCs use n-butanol as working fluid and typically have lower particle detection limits in the range between 2.5 and 10 nm (Stolzenburg, M. R., & McMurry, P. H. (1991). Aerosol Science and Technology, 14(1):48-65). Given the fact that n-butanol CPCs are operated at fixed temperatures, the performance towards the detection of even smaller particles may be optimized by choosing appropriate temperature settings.

Until now the temperature dependence of heterogeneous nucleation of n-butanol vapor on nanoparticles in a size-range down to 2.5 nm was not investigated. A topic, however, that is worth examining since it gives information on the saturation ratio which is needed to activate particles in this size range. Results of earlier experiments with water vapor nucleating on silver particles have shown a theoretically unpredicted maximum in the onset saturation ratio as a function of temperature (Kupc et al. (2013). Aerosol Science and Technology, 47(9):i-iv). Further studies on the nucleation of n-propanol on sodium chloride particles in the temperature range from 262K to 287K indicate a reverse trend of the onset saturation ratio compared to the Kelvin equation (Schobesberger et al. (2010). ChemPhysChem, 11:3874–3882). Due to the close chemical similarity of n-propanol and n-butanol, and the common use of n-butanol as a working fluid in commercial CPCs, the temperature dependence of heterogeneous nucleation of n-butanol on Ag and NaCl particles is investigated in this study.

We have measured the onset saturation ratio of n-butanol depending on nucleation temperature with the size analyzing nuclei counter SANC (Wagner et al. (2003). Phys. Rev. E67:021605-1). NaCl and Ag seeds generated by a Scheibel-Porstendörfer (1983) aerosol generator in the size range from 2.5 to 9.0 nm were used as condensation nuclei. We found an inverse temperature dependence for the heterogeneous nucleation of n-butanol on sodium chloride particles similar to the n-propanol data from Schobesberger. To rule out humidity effects the air supply of the tube furnace was exchanged, dried compressed air was replaced by synthetic air with < 3ppm-mol humidity. Thereby the found inverse temperature trend disappeared. This indicates that the driving force for the inverse temperature dependence is the increased relative humidity at lower temperature.

Additional to the SANC measurements, we determined the cut-off diameter at variable condenser temperature and air humidity, with constant ΔT between saturator and condenser, for a commercial n-butanol CPC. Thereby, lower D50 cut-off diameter for NaCl and Ag particles at reduced temperatures could be observed. Accordingly, by lowering the condenser temperature and hence nucleation temperature of a butanol CPC, the counting efficiency can be increased significantly for both, NaCl and Ag seeds – with a stronger response for NaCl particles. Furthermore, the effect on detection efficiency of different relative humidity was investigated; results of earlier studies have indicated different humidity dependence for sodium chloride and silver nanoparticles (Gilmore, J. S. (2002). Atmospheric Research, 62(3–4):267-294).

By merging the experimental results of the SANC and commercial condensation particle counters combined with theoretical predictions we are able to examine the heterogeneous nucleation of n-butanol on different seeds in greater detail. The findings are of immediate relevance for nanoparticle detection in CPCs and raise questions on the fundamental mechanisms leading to this behavior.

10AP.3

Measurement of the Size Distribution of Stable Clusters during Silane Pyrolysis in a Helium Atmosphere. MIGUEL VAZQUEZ PUFLEAU, Yang Wang, Elijah Thimsen, Pratim Biswas, *Washington University in St. Louis*

Nucleation is the first stage required for gas phase species to become solid or liquid. It is highly relevant for both industrial and environmental applications, yet the phenomenon is not well understood. This has constrained optimal design of efficient processes in numerous industries including semiconductors, photovoltaics and ceramics, and limited the accuracy of weather modeling and forecasting. Current approaches to describe the initial stages of aerosol formation are based on the classical nucleation theory (CNT), which predicts the existence of a critical size above which particles are stable and grow larger and below which particles are unstable and can easily break apart. CNT was conceived for physical systems. But, by analogy of principles, the concept of chemical equilibrium as given by the free Gibbs energy has been used to predict critical nucleus sizes. For silane, at given process conditions, stable silicon hydride molecules, with a given amount of silicon atoms, have been determined based on ab initio calculations. However, experimental evidence of the mobility of such silicon clusters produced during silane pyrolysis was not available.

In the present work, we measured for the first time the mobility of sub nm silicon hydride stable clusters using a half mini differential mobility analyzer. The clusters were produced during silane pyrolysis at different conditions in a flow reactor. The clusters measured at different temperatures displayed a peak at around 0.75 nm mobility. The effect of residence times was also assessed. Transmission Electron Microscopy (TEM) characterizations and particle size analysis were undertaken to provide insights into the larger particle mode at conditions with partial silane conversion in which other standard online characterization instruments could be biased due to the unreacted precursor interfering with the measurement. In addition, a dependence of stable cluster abundance as a function of process parameters was observed, analyzed and compared with silicon hydrides predicted to be stable from ab initio calculations reported in the literature, showing good agreement.

MVP and YW contributed equally to this work.

10AP.4

Enhanced Raman Spectroscopy of Individual Aerosol Particles. VASANTHI SIVAPRAKASAM, Matthew B. Hart, Jay D. Eversole, *Naval Research Laboratory*

This presentation provides new data from an on-going investigation of the addition of metallic nanoparticles (MNPs) to micron-sized aerosol particles for the purpose of developing and characterizing enhanced Raman spectroscopic signatures that can serve to identify the aerosol material on a particle-by-particle basis. While Raman spectroscopy is a well-established method of chemical identification, typical spontaneous molecular cross sections are too low to permit application to in-situ, on-the-fly interrogation of aerosol particles in the picogram to nanogram mass range. Consequently, the goal of rapidly discriminating among a population of aerosol particles would require some degree of enhanced optical signature. We have investigated enhanced Raman scattering (both its intensity and spectral form) from single particles in which MNPs have been either dispersed within the particle material or deposited on the particle surface. The mechanisms giving rise to Raman enhancement in this type of system are essentially the same as the more familiar arrangement of surface enhanced Raman spectroscopy (SERS).

We recently observed enhancement factors > 10^5 in single aerosol particles with dilute concentrations of rhodamine 6G (R6G) when these particles were combined with small quantities of gold MNPs (Sivaprakasam et. al. 2017[1]). These experiments were conducted with the use of a linear electrodynamic quadrupole (LEQ) particle trapping chamber so that aerosol particles could be generated as charged droplets with controlled composition and maintained in fixed position in the chamber. Once the solvent liquid evaporated composite residue particles remain suspended in the trap. This experimental system provides a capability to study particles and obtain data over extended periods of time (up to hours). Particles were generated under identical conditions both with and without the presence of MNPs, permitting a direct comparison of spontaneous Raman and MNP-enhanced Raman spectra from particles of the same size and composition. Additionally, droplets of neat ethyl cinnamate served to provide an absolute external reference for calibrating our Raman cross section measurements. Our initial study of R6G-containing particles showed excellent repeatability for both spectral response and enhancement factors, and dependences of the enhanced Raman scattered light on MNP concentration and R6G concentration were determined.

Our most recent results, on micro-droplets of adenine and also of microspheres of polystyrene latex (PSL) and polymethyl methacrylate (PMMA) will be presented and discussed.

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10AP.5

Interpreting the Kinetics of Ballistic-to-Diffusive Transition Using Directional Statistics. PAI LIU, William Heinson, Benjamin Sumlin, Rajan K. Chakrabarty, *Washington University in St. Louis*

We demonstrate a new method to interpret the rate of ballistic-to-diffusive (BD) transition in stochastic motion commonly observed in many physical systems. The correlation between successive steps of the motion is parametrized using a wrapped Cauchy distribution (WCD) that governs the probability distribution of the tracer's turning angle. With increasing timescale, the distribution evolves from a delta function to a uniform distribution, marked by a decrease in the shape factor of WCD. This trend agrees with BD transition behavior revealed from the scaling law between the mean-squared displacement and time. We next propose an analytical solution to the decrease in the shape factor which accurately predicts the transition rates. We conclude this work with simple mathematical equations that relate three parameters of the motion: time, exponent of the spatial-temporal scaling power-law, and the shape factor of WCD.

10AP.6

Experimental Studies on the Charge Distribution of Aerosol Particles from a Fluidized Bed Aerosol Generator. QUN ZHOU, Cai Liang, Lunbo Duan, Xiaoping Chen, Daoyin Liu, Changsui Zhao, *School of Energy and Environment, Southeast University*

Fluidized beds have been used for generation of aerosols in many applications for many decades.However,aerosols obtained high level electrostatic charge and different polarity charge as a result of continuous particle-particle and particle-generator wall contacts will result in agglomeration and their severely adhesion on the wall.It is necessary to see into the electrostatic charging mechanism in the fluidized bed aerosol generator.In this study,particles of different materials were fluidized in a 0.1 m in diameter column under atmospheric conditions for 1h,the size distribution,net charge and charge distribution of particles in different region(bulk region and wall region) were determined by an online Faraday cup measurement technique and wind sifting method.We founded that positively and negatively charged particles both existed within each region,and revealed the relationship between particle charge distribution and its size distribution.A new mechanism was proposed to explain the charged particle migration towards the column wall.

10AP.7

The Hygroscopicity of Particles That Carry Differing Charges and Their Impact on Tandem Differential Mobility Analyzer Measurements of Biomass Burning Aerosol. CHRISTOPHER OXFORD, Rajan K. Chakrabarty, Brent Williams, *Washington University in St. Louis*

Biomass burning aerosol (BBA) constitutes a significant fraction of atmospheric aerosol and impacts health, visibility, and radiative forcing. The nature and scale of these impacts are influenced by the size distribution of the aerosol, which is governed by hygroscopicity at elevated (90%) relative humidity. Characterization of BBA during the second Fire Lab At Missoula Experiment (FLAME-II) determined that BBA with high inorganic concentrations exhibited bimodality rather than a singular hygroscopicity[1]. Bimodal hygroscopicity could be caused by condensation of hydrophilic inorganics, release of hydrophobic soot aerosol, presence of non-spherical morphologies, and condensation of volatile organic compounds with low hygroscopicity. Conclusions from FLAME-II attribute the bimodality to externally mixed BBA at a given diameter[2]. Other authors, using different fuels, attribute differences in BBA hygroscopicity to non-spherical morphologies[3].

Hygroscopicity can be determined with a Tandem Differential Mobility Analyzer (TDMA), which measures changes in mobility size due to the condensation of water on selected particles. TDMA inversion routines assume the selected particles are singly charged[4,5]. Investigating sizes smaller than the mean of the log-normal size distribution (μ) could select a population of multiply-charged particles, violating the single charge assumption. Therefore, TDMA users must choose a diameter larger than μ[6] to reduce error in the singly-charged assumption. However, μ during chamber studies can often exceed 150 nm, and the upper measurement limit of many TDMAs prevent determination of the final diameter of high growth particles larger than a dry diameter of 200 nm. The measurement limits and assumption limits can create a narrow window of available mobility sizes.

We emitted primary organic aerosol from the flaming combustion of grasses sourced from Western Montana and employed a Centrifugal Particle Mass Analyzer (CPMA) in combination with the TDMA to determine separately the hygroscopicity of particles that carry single, double, and triple charges. To address the possibility of morphology as a contributing factor to bimodality, we also obtained Transmission Electron Microscopy (TEM) images of the aerosol. We show that the individual charges do not move equally in mobility space allowing the size distribution to influence the measured hygroscopicity.

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10AP.9

Using Electron Tomography to Better Characterize the Fractal Morphology of Aerosol Aggregates. CHENCHONG ZHANG, Pai Liu, William Heinson, Qing Li, Jingkun Jiang, Rajan K. Chakrabarty, *Washington University in St. Louis*

Freshly emitted soot particles normally demonstrate complex fractal-like morphologies which could significantly influence atmospheric radiative forcing and aerosol-cloud interaction. An accurate parameterization of the morphology of these particles is an essential prerequisite for evaluating their role in global radiative forcing. However, retrieving the complete morphological information in 3-dimension (3-d) remains a challenging task due to information loss incurred during image processing of projected electron microscopy images of soot. As a result, the currently adopted morphological descriptors for soot commonly assume the monomers to be point-contacted and equally-sized spheres, which deviate considerably from their true morphology especially when considering their unevenly coated surfaces and sintering. Here, we demonstrate a novel 3-d reconstruction algorithm for soot aggregates using the electron tomography technique. Particle tomograms, retrieved from a tilt-series of transmission electron images, were used to generate 3-d geometric models of soot aggregates after proper rescaling. Our methodology precisely captures the detailed morphological information of the particles, for example, the exact shapes of primary particles and degree of sintering. We calculated the structure factor of the reconstructed models by performing Fourier transform of the voxel density autocorrelation function. We compare the structure factors of our 3-d reconstructed model with those of aggregates simulated using the classical 3-d off-lattice diffusion limited cluster-cluster aggregation technique. We anticipate our findings to improve upon the morphological descriptors of soot and fractal-like aggregates produced from various combustion processes.

10AP.10

Mobility of Nanofiber, Nanorod and Non-spherical Nano-agglomerates in Gases. LIN TIAN, Goodarz Ahmadi, Jiyuan Tu, *RMIT University*

Accurate measurement and classification of nanoparticles are in great need in context of fast development of nanotechnology. Nanoparticles frequently appear in non-spherical forms such as long aspect ratio nanofibers, nanotubes, and irregular nano-agglomerates. While well-developed classical studies were mainly in continuum regime with spherical particles, dynamics of non-spherical nanoparticles is still not fully understood. In this study, orientation averaged mobility of the nanofiber and nanorod is examined by methods of Brownian diffusion theory, a combination of the collision limited reaction rate theory and the bipolar diffusion charging analysis, and empirical predications from measurements. The study leads to the discovery of a surface dominated mobility for nanoparticles with Knudsen number greater than 5 ($Kn > 5$). In view of the extreme relative length scales between particle size and gas mean free path, particles of all morphologies can be viewed as point collision and therefore the equivalent surface mobility diameter is reasonably justified. As expected, the accuracy of this approximation reduces as the Knudsen number decreases. When $Kn < 0.1$, the study shows that the particle morphology starts to play an important role.

10BA.1

Measuring Changes in Bioaerosol Fluorescence over Time with the WIBS. ELIZABETH CORSON, Jonathan Eshbaugh, *JHU/APL*

Exposure of biological aerosols to atmospheric processing may result in changes in viability and spectral signatures. Many instruments rely on particle fluorescence measurements to detect biological aerosols. Therefore, understanding changes in fluorescence signature over time is critical for accurate bioaerosol detection. The Wideband Integrated Bioaerosol Sensor (WIBS-4A, Droplet Measurement Technologies Inc.) measures particle fluorescence at two excitation wavelengths, 280 nm and 370 nm, and two emission spectra, 310-400 nm and 420-650 nm. This multichannel approach to fluorescence measurement produces informative data about the state of a bioaerosol population over time. Two bioaerosol aging campaigns were completed using a rotating drum to maintain an aerosol population and expose the aerosol to atmospheric processing effects, such as water vapor, ultraviolet light, and ozone. The aerosol was measured over time using a WIBS-4A and an Ultraviolet Aerodynamic Particle Sizer (UVAPS, TSI Inc.). Changes in fluorescence signatures over time were observed in a vegetative bacteria and a protein, especially when those aerosols were exposed to ozone and water vapor. Fluorescence data will be presented with an emphasis on methodology for investigating bioaerosol fate and how to interpret raw WIBS data in this context.

10BA.3

Bacterial and Fungal Aerosol Emissions from Different Land Types. XINYUE LI, Maosheng Yao, *Peking University*

Human activities are changing the land-use types and patterns continuously, and also affecting the interaction between land and atmosphere in the fields of physics, chemistry and biology. As a significant source of atmospheric bioaerosols, microorganisms from land emission have noteworthy influence on regional ambient air quality, public health and climate change. However, the studies about the characteristics and variations of microbial aerosols in various types of land-use are still not sufficient. Here we report a study of microbial aerosols in several different land-use areas in an urban setting including garden, forest, lakes, wet land, farmland, livestock farm, sewage treatment plant, main roads, smeltery and bare land. Samples collected with a new high flow portable biological aerosol sampler (HighBioTrap) developed by our group. Plate cultivation and real-time quantitative PCR were respectively used to quantitatively analyze the concentrations of culturable microorganisms and total microorganisms. The characteristics of microbial community structures in different areas were also analyzed with high throughput gene sequencing: 16s rRNA for bacteria and ITS for fungi. Our results showed that there were differences in their concentration and compositions of microbial aerosols among different land-use types. The results showed that the livestock farm had the highest bacterial aerosol concentration levels, followed by main roads, smeltery, sewage treatment plant, lakes, garden, forest, bare land, farmland and wet land. The rates of bacteria and fungi aerosols (B/F) suggested microbial community structures varied from 21.7 (in forest) to 0.8 (upon bare land). Sequencing results showed there were significant differences in their microbial aerosol structures. For fungi community, the *Tremellales* and *Pleosporales* were detected to dominate in most sites, but a large proportion of fungi was unclassified. This work researched the features of microbial aerosols from multifarious land-use types more comprehensively, found significant diversity of microbial aerosols among different types of land-use. It provided more valuable views to identify the ambient air quality and evaluate population health risks exposure to urban micro-bioaerosol.

Keywords: Microbial aerosol, Land-use areas, Airborne microorganisms, Bacteria, Fungi

10BA.4

Atmosphere Bioaerosols in Different Micro- Environments of Megacity of Lagos, Nigeria: Relationship between Ambient Concentrations, Volatile Organic Compounds and Weather Parameters. EMMANUEL OLUMAYEDE, Chukwebe Ojiodu, *Federal University Oye - Ekiti*

This objective of this study is to investigate the relationship between outdoor concentrations of bioaerosols, Volatile Organic Compounds and meteorological parameters in different microenvironments of Mega city, Lagos Southwest Nigeria, so as to ascertain the influence of these factors on bioaerosol levels. Airborne bacterial, volatile organic compounds (VOCs) and weather parameters were continuously monitored for the period of one year at two weeks intervals. Ambient aerosol samples were collected using a low volume handy sampler operated at flow rate of 2 L min–1. Meanwhile, the VOCs were collected by passive sampler (ORSA 5). Samples were collected at a height of ~1.5–2 m above the ground level for sampling to simulate exposure in the human breathing zone. The adsorbed VOCs were desorbed with carbon disulphide (CS2) and the solution analyzed using Gas Chromatography (GC) fitted with Flame Ionization Detector (FID). The results showed that 15 VOCs are quantified, with spatiotemporal pattern of high concentrations in winter. The total mass concentrations of identified organic aerosols range from 4.2 x 102cfu/m3 (Ilupeju) to 7.8 x102cfu/m3 (ojota). The levels of aerosols were correlated with levels of atmospheric volatile organic compounds and meteorological parameters using generalize linear model. The relationship was linear and significant, with R2 and P value being 0.978 and < 0.01.

10BA.5

A Clinic Table to Prevent Aerosol Transmission Based on Wind Curtain. HUA QIAN, Jin Ye, Jichen Ji, Xiaohong Zheng, *Southeast University*

Aerosols transmission is a main vehicle of respiratory infectious diseases. Literatures showed that the risk of droplet borne and airborne is much higher than long range airborne. The fact encourages us to find a way to cut off short range droplet borne and air borne routes. However, traditional partition method also cut the information exchange route and bring unpleasant feeling of patients. That method is not suitable to use in clinic table, where doctor need to identify diseases through asking and observing infectious diseases.

Based on win curtain technology, a clinic table to prevent aerosol transmission diseases was proposed. Computation fluid dynamics (CFD) was employed to verify the performance of the clinic table and optimize the parameters of the clinic table. Velocity field, temperature field , contaminants concentration field, and dispersion of aerosol was investigated for different parameters of the clinic table. Results showed that the table was very efficient to cut off the aerosol transmitted route. The exposure of doctor to the patients with wind curtain is less one tenth than that without wind curtain. The optimized wind speed is 3m/s. The reason better than 2m/s is due to strong wind is better to cut off the routes. The reason better than 4m/s is due to jet entrainment. And the optimized supplied angle is 20^{o}.

10BA.6

Bioaerosols Abundance Variability through Cloud Decks across Multiple Environments during BOAS Campaign.

ARNALDO NEGRON-MARTY, Natasha De Leon-Rodriguez, Natasha Hodas, Matthew Coggon, Kelvin Bates, Armin Sorooshian, Haflidi Jonsson, John Seinfeld, Richard Flagan, Kostas Konstantinidis, Athanasios Nenes, *Georgia Institute of Technology*

Primary biological aerosol particles (PBAP), also known as *Bioaerosols*, are emitted into the atmosphere from soil or plants in terrestrial environments, or from the sea surface microlayer in marine environments. Once they reach the planetary boundary layer, meteorological factors {e.g. UV radiation, temperature, wind speed and relative humidity (RH)}, particle size and composition will affect the bioaerosol viability and eventually lifetime. Bioaerosols can act as cloud condensation nuclei (CCN) or as ice nucleating particles (INP), and may affect cloud microphysics. We studied the abundance and variability of PBAP in and above cloud capped boundary layers onboard the CIRPAS Twin Otter using the Wideband Bioaerosol Integrated Sensor (WIBS) (Perring et al., 2015; Ziemba et., al 2016; Twohy et al., 2016) and a wet-wall cyclone sampler (SpinCon II) during the BOAS 2015 campaign. In addition, WIBS-4A sampled through a Counterflow Virtual Impactor (CVI) in cloud to study the presence and population composition of bioaerosols in cloud droplets. WIBS-4A data was used to quantify the abundance of FBAP and SpinCon II samples were post-processed by flow cytometry (FCM) to quantify the total PBAP concentration. Results show a persistent enrichment of bacteria in the detrainment region of the boundary layer, by which the total PBAP can constitute up to 30% of the total coarse mode particles above 500nm, with important implications for the biogeography of PBAP. Results suggest that a substantial amount ($\sim 10^4$ m^{-3}) of sea-spray aerosolized bacteria reaches cloud formation relevant altitudes. The abundance variability of WIBS-4A FBAP categories (e.g. A, B, C, AB, BC AC, ABC) below cloud, above the boundary layer and in the cloud drop residuals are used to study the lifecycle of bioaerosols within the boundary layer.

10BA.7

Long-Range Transport of Biogenic Aerosols Monitored at the Cape Verde Atmospheric Observatory (CVAO) from 2015 to 2016. DOUGLAS MORRISON, Martin Gallagher, David Topping, Ian Crawford, Michael Flynn, Katie Read, Paul Kaye, Virginia Foot, *University of Manchester*

Long-range transport of biogenic aerosols can have important ecological consequences. It can introduce species and diseases to new environments, shift ecosystem dynamics and lead to animal and human diseases, including common respiratory problems in humans. They can damage crop yields, leading to food insecurity, and may also affect climates by influencing cloud and precipitation formation. It is therefore important to understand the mechanisms, activities and conditions by which it can occur and to quantify, through observational studies, the magnitude and frequency of such contributions. On the eastern coast of the island of São Vicente, the Cape Verde Atmospheric Observatory (CVAO) monitored bioaerosols from October 2015 to September 2016 using a WIBS 4M UVLIF bioflureoscent aerosol spectrometer. Using a newly developed UVLIF discrimination algorithm, analysis showed significant seasonal trends in concentrations over the 11 months, with a distinct peak during December. As the relative number of total aerosols does not fully explain this rise, it is concluded that the elevated bioaerosol concentrations during this period were the result of long range transport following biomass burning in Western Africa. Seasonal back trajectory analyses were undertaken to support this conclusion to determine and confirm the bioaerosols source region, primarily the West African continent. Hierarchical cluster analysis is also used on the single particle UVLIF signatures to identify the probable class of bioaerosols observed and to relate these to seasonal source changes. The aim of this study is to distinguish contributory sites or activities, natural or anthropogenically influenced, on bioaerosol dispersion and to quantify their wider impacts.

10BA.8

A Study on Biological Constituents of PM1 over Semiarid Region of Indo-Gangetic Basin. ROHINI SINGH, Ranjit Kumar,
DEI, Dayalbagh, Agra, India

Air is filled with numerous aerosols with biological origin called as bioaerosol. Exposure to bioaerosols has been linked with climate change and adverse effects on health. They cause toxic reactions and infections, hypersensitivity, asthma, pneumonitis, allergens etc. A few studies on microbial constituents of aerosols are reported but none on microbial components in PM_1 (fine particles). The present study deals with mass concentration of PM_1 over semiarid region of Indo-Gangetic basin and microbial composition, concentration, and regional diversity. The mass concentration PM1 is in the range of 10-50 µg m^{-3} which can be considered as high although the standard for PM_1 is not set yet. The concentration (colony forming unit per cubic meter) of total microbial components (TMC), bacterial components (BC) and fungal components (FC) are determined and morphological and biochemical characterization has been carried out. The concentration of TMC is well below the reported range 1-1000 cfu m^{-3}. The bacterial concentration is higher than fungal concentration. The Gram –ve bacteria is more than Gram +ve. Coccus is dominant over Bacillus. Some of the identified bacteria are pathogenic in nature. Among fungi the Aspergillus is dominated followed by Penicillium, Torulla, Alternaria, Trichothecium, Mucor, Rhizopus, and Fusarium. The concentration of bacteria and fungi is influenced by meteorological conditions. The correlation and regression analysis reveals bacteria are significantly correlated with temperature and fungi are with relative humidity.

10BA.10

Modulation and Resilience of the Metabolome of Pseudomonas graminis, a Cloud Bacterium, Facing H2O2 Atmospheric Stress. Nolwenn Wirgot, Marie Lagree, Mounir Traikia, Cyril Jousse, Isabelle Canet, Martine Sancelme, Pierre Amato, Ludovic Besaury, Bernard Lyan, ANNE MARIE DELORT, *Université Clermont Auvergne*

In cloud waters microorganisms are metabolically active although they are exposed to very strong stresses, especially due to the presence of reactive oxygenated species, including H_2O_2 and radicals [1,2]. In order to understand how microorganisms can modulate their metabolism facing H_2O_2 stress [3], we have investigated by a metabolomics approach the response of a *Pseudomonas graminis* strain, isolated from cloud waters, to hydrogen peroxide exposure. For this purpose *P. graminis* cells were incubated in microcosms containing artificial cloud waters in the presence or absence of H_2O_2. Metabolites were extracted at two time points (50 min and 24 h) that were important regarding the evolution of ATP cellular content and H_2O_2 degradation over time. These bacterial extracts were analyzed by LC-MS and 1H-NMR using the Metabolic Profiler® facility (Bruker). Metabolic profiles were converted into matrices and statistical analyses (PCA, PLS-DA) were performed; key markers of this oxidative stress were identified by 2D NMR and LC-MS-Orbitrap.

At time 50 min, when H_2O_2 was still present in the incubations, the bacteria adapted and modulated their metabolome facing this stress. The major metabolic pathways of *Pseudomonas graminis* (13b-3) impacted by the presence of hydrogen peroxide were the carbohydrate pathway, glutathione, energy, lipid and amino-acid metabolisms. Unexpectedly, the concentration of a few dipeptides containing mainly Ala, Val, Leu (Ile) was also highly modified in the presence of H_2O_2. These dipeptides are reported here for the first time as biomarkers of oxidative stress. Interestingly, at time 24 h, when H_2O_2 has been completely biodegraded by the cells, no more significant difference was observed between the metabolites of exposed and non-exposed cells to H_2O_2. This shows the resilience of this bacterium metabolome after H_2O_2 stress exposure.

These results are discussed in terms of impacts on cloud chemistry.

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10BA.11

Impact of Composting Recycled Manure Solids on Bioaerosols in Dairy Farms. KARINE DUQUETTE-LOZEAU, Joanie Lemieux, Valérie Létourneau, Sébastien Fournel, Caroline Côté, Stéphane Godbout, Caroline Duchaine, *CRIUCPQ, Université Laval, Canada*

Using recycled manure solids (RMS) (solid fraction separated from fresh cow manure that is thermally conditioned) bedding for dairy cows is a practice gaining rising interest from Canadian dairy producers. However, impact on human health of spreading this material in stalls remains unknown. In the present study, the influence of the composting method used in producing the RMS on the air quality was evaluated in environmentally controlled and confined experimental chambers. Four composting approaches were tested: SW) static; TW) turned daily; DC24) static after 24 h in a drum composter; DC72) static following 72 h in a drum composter. Air samples were taken using Coriolisµ Biological Air Sampler (200 L/min, 10 min, Bertin Corp.) and a SASS® 3100 Dry Air Sampler (300 L/min, 10 min, Research International) at days 0 (while loading of the containers in chambers with the solids), 5 and 10. The experimental set-up aimed to mimic worker's exposure up to 10 days following the spreading of the RMS in manure composting facilities. Airborne microorganisms were analyzed by culture (mesophilic bacteria and fungi, thermotolerant fungi) or by qPCR for total bacteria (16S rRNA), *Penicillium/Aspergillus* (ITS1), *Klebsiella pneumoniae* (phoE), *Aspergillus fumigatus* (ITS1) and *Saccharopolyspora rectivirgula* (16S rRNA).

At day 0, as RMS were pilled, microbial concentrations were higher than ones observed on days 5 or 10, essentially because of the loading activity. However, some composting techniques were associated with low microbial concentrations and thus, are preferable with regards to occupational exposure. At day 0, SW treatment showed the lowest concentrations of airborne culturable mesophilic bacteria and *Penicillium/Aspergillus*. TW treatment was characterized by the lowest airborne culturable mesophilic fungi and total bacteria. Over time (days 5 and 10 after RMS was loaded), TW and SW composting methods also showed the lowest airborne microbial concentrations. For culturable thermotolerant fungi concentration as well as *K. pneumoniae*, *A. fumigatus* and *S. rectivirgula* concentrations, quantified by PCR, no significant difference were observed over time between composting methods.

In conclusion, SW seems to be the composting method to privilege in order to minimize occupational exposure to airborne microorganisms. In the next few months, other airborne respiratory pathogens will be quantified from the same air samples and the impact on air quality of spreading and using RMS as cow bedding will be studied in commercial dairy barns.

10BA.12

Influence of Occupant Characteristics on Indoor Microbiome. DAHAE SEONG, Shamia Hoque, *USC*

Indoor air is an evolving environment that changes with time, occupant behavior, building interior, and ventilation design. Numerous studies have investigated the impact of surrounding environments to determine how they influence the indoor conditions and how they interact with each other. Recent studies have revealed that human activity and occupancy highly influence indoor microbial composition and concentration. The influence of male to female gender rations has been observed at university dormitories and restrooms. Some microbes have been revealed to show a gender signature, such as *Corynebacterium* and *Lactobacillus*, typically identified at specific gender assigned rest rooms. Although indoor microbes have been widely studied at diverse locations we are still trying to assign sources to the components of the microbiome. In this study we look at the impact of different age groups, room function and seasonal changes. Sampling is being conducted across different school buildings at different locations. The schools are classified into elementary school, high school, and university. The objective of the study is to investigate how the microbial composition and their concentrations vary (if any) with different age groups and different usage of room. Since sampling is being conducted over a long period of time, the effects of weather will also be assessed.

The age groups are classified into three groups, childhood (4 to 11 years old), adolescence (12 to 18 years old), and adulthood (older than 18 years). Ambient air and surfaces are sampled. Bacteria from ambient air are collected through a passive sampling using Petri dishes filled with nutrient agar. Surface samples are collected using sterile swabs. Samples have been being collected on October 2017, December 2017 and January 2018. Samplings at all schools were conducted in the classroom, boy's and girl's locker rooms, and libraries which students consistently use, but have a different occupancy rate and gender-ratios. The presence and persistence of microbes can be influenced by the surface types present. Since the most predominant surface materials in the schools were wood, plastics, and metal, three different materials were selected as swab locations. HVAC systems were operating during the sampling time.

Analysis of the results show that inhalable particles under 0.5 µm were dominant in both locker rooms. The number of particles in the boy's locker room was much higher than the girl's locker room sampled at high schools. The microbial concentration in the samples from both high school and university locations show that that male-occupied rooms had more variation in the microbiome than rooms routinely used only by females (male and female locker rooms). This was also observed in another study and this could be because men scattered skin cells more than women. Predominant indoor microorganisms, *Staphylococcus*, *Micrococcus*, and *Bacillus*, were identified in all the locker rooms and classrooms. At all sampling locations, except one classroom, *Staphylococcus* was dominant. *Micrococcus* sp., *Bacillus* sp., *Rhodotorula* sp., and *Aerococcus* were the other species identified. The sampling was conducted during a cold spell. The weather influence was noticed on the microbial composition which included *Rhodotorula* sp., and *Aerococcus*. These species grow more at lower temperature than others such as *Bacillus* which was also identified. For a more in depth understanding of the age impact, more samples from schools with children in the age groups of 4 – 11 have to be collected. The ultimate goal is to determine if there is a correlation between the microbiome diversity and quantity to occupant and building characteristics.

10BA.13

Ice Nuclei Activity of Fungal Spores Collected in the Metropolitan Area of São Paulo, Brazil. ANA PAULA MENDES EMYGDIO, Dulcilena de Matos Castro Silva, Ricardo Matheus Pires, Fabio Luiz Teixeira Goncalves, Maria de Fatima Andrade, *University of Sao Paulo*

Bioaerosols are related to respiratory diseases and also have an impact on several atmospheric processes, such as scattering and absorption of radiation and they can influence on cloud formation being cloud condensation nuclei (CCN) and ice nuclei (IN). Several studies have been performed to determinate the capability of the bioaerosol to be ice nuclei, specially bacteria and fungal spores. The aim of this work was to evaluate the ice nuclei activity (INA+) of several fungal spores present in the atmosphere of Sao Paulo. To achieve these objectives, fungal spores were collected in the metropolitan area of São Paulo with two methodologies: using the impactador "AR MAS 100-ECO" (Merck, FR) (250 liters) with modified DRBCm Dichloran Rose-Bengal culture media and extract with ethanol solution; and for the Basidiomycota group, fruiting bodies were collected in the forest fragment (Parque Estadual das Fontes do Ipiranga) and the spores were extracted using the spore print methodology. After the collection, freezing tests were performed using a thermostatic bath with ethanol and water, the amount of spore in each solution was determinate with a Neubauer chamber. A total of 32 drops with 10µl from each of the 13 fungal types were tested considering three different dilutions including: *Henningsia brasiliensis (Hb), Macrolepiota sp. (M), Ganoderma australe (Gs), Dichomitus setulosus (Ds), Flaviporus liebmanii (Fl), Pycnoporus sanguineus (Ps), Fusarium sp. (F), Trichoderma sp. (T), Aspergillus sp. (A), Aspergillus niger (An), Antrodiella liebmannii (Al), Ceriporia xylostromatoides (Cx), Arbortiporus fractipes (Af).* Ultrapure Milli-Q water was also tested for comparison. In all tests the ultrapure Milli-Q water starts to freeze below -20ºC. The total volume of spores suspended for the three dilutions was (i) $10^{+6}/10^{+7}$ spores/mL, (ii) $10^{+5}/10^{+6}$ spores/mL, (iii) $10^{+5}/10^{+4}$ spores/mL. Only the *Gs* had a dilution factor of (i) 10^{+4} spores/mL, (ii) 10^{+3} spores/mL and (iii) 10^{+2} spores/mL. The higher initial freezing temperature for all spore tested was -9ºC for *M* and *Af* and the lower initial freezing temperature was -22ºC for *T* considering the most concentrated solution (i -10^{+7} spores/mL). The initial freezing temperature increased as more concentrated the solution. The initial and final temperature of freezing and the first and last cumulative ice nucleation activity per spore according to the calculation of Vali (1971) for the (i) dilution were: *Hb* (-14ºC/-25ºC; 1.9×10^{-05}; 1.1×10^{-03}), *M* (-9ºC/-25ºC; 1.6×10^{-6}), *Gs* (-11ºC/-25ºC; 1.3×10^{-4}), *Ds* (-14ºC/-25ºC; 3.3×10^{-7}; 8.5×10^{-6}), *Fl* (-11ºC/-25ºC; 2.9×10^{-6}), *Ps* (-14ºC/-25ºC; 3.3×10^{-8}), *F* (-16ºC/-23ºC; 6.7×10^{-7}; 2.4×10^{-5}), *T* (-22ºC/-23ºC; 1.8×10^{-7}; 3.6×10^{-7}), *A* (-13ºC/-23ºC; 9.6×10^{-7}; 4.2×10^{-5}), *An* (-19ºC/-23ºC; 2.4×10^{-7}; 8.0×10^{-6}), *Al* (-15ºC/-21ºC; 3.4×10^{-7}; 3.7×10^{-5}), Cx (-14ºC/-21ºC; 1.4×10^{-6}), *Af* (-9ºC; 4.9×10^{-6}; 5.3×10^{-4}). The freezing temperature of all spores tested indicates that they could contributed to a heterogeneous ice cloud formation, since all spores freeze in a temperature warmer than -19ºC (except for the *T*) and the ultrapure Milli-Q water freeze in temperature colder than -20ºC. However, only the *Macrolepiota sp.* and the *Arbortiporus fractipescan* presented significant ice nuclei activity with this experimental design. It should be considered that factors other than temperature should be accounted for the heterogeneous ice cloud formation, such as the size of the spore and the height needed to reach the temperature required for freezing.

10BA.14

Investigation of Bioaerosol Charge Levels Indoors Using the Rutgers Electrostatic Passive Sampler (REPS). SYDONIA MANIBUSAN, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

Previous studies have demonstrated the Rutgers Electrostatic Passive Sampler (REPS) as a novel and effective method for collecting bioaerosol samplers. REPS uses specially arranged and permanently polarized ferroelectric films to electrostatically attract charged airborne particles and deposit them on a film for easy elution and analysis. The REPS device’s method of electrostatic deposition of bioaerosol particles onto film offered a unique opportunity to study the polarity of bioaerosol particles.

The aim of this study was to determine the effect of seasonality on bioaerosol charge using a direct-plating analysis method. REPS devices were used to sample indoor residential environments during the summer and winter over 48-hour intervals. The devices were collocated with an active bioaerosol sampler, the SAS Super 180 Microbial Sampler (Bioscience International, Inc., Rockville, MD), and passive sampling using agar settling plates. The SAS sampler and settling plates sampled at 6 intervals for 3 minutes and 2 hours, respectively. REPS films with the collected microorganisms were either press-plated or eluted into the water for analysis. The press plate method involved applying one side the film directly onto two identical square Tryptic Soy Agar (TSA) or Malt Extract Agar (MEA) plates for bacteria and fungi, respectively. Both the film position and charge (+ or -) of the pressed film face were recorded for each sample plate. The elution method of the collected microorganisms included vortexing and sonication of the entire REPS sampler into 40mL of autoclaved milli-Q water followed by spreading 100µL of the elution liquid onto TSA and MEA plates. All plates were incubated at room temperature and counted for 5 consecutive days.

Passive sampling using the REPS device found average bioaerosol concentrations of 0.784 CFU/cm^{2}h in the summer and 0.131 CFU/cm^{2}h during winter for study location. Active sampling by SAS 180 yielded average culturable bioaerosol concentrations of 291.9 CFU/m^3 of bacteria and 109.1 CFU/m^3 fungi during winter. The data from summer months showed that almost 90% of bacteria and fungi were attracted to the positively polarized film face, i.e., they carried a negative charge; no significant difference among bioaerosols due to charge was observed during the winter months. This approach to bioaerosol sampling provides a novel method of observing the different impacts of the season and other factors that may affect the behavior and composition of bioaerosols in indoor environments. The study will be expanded to include additional and more diverse indoor environments.

10BA.16

The Effects of Alpha-pinene and Toluene in the Presence of UV, Ozone, and Humidity on Bioaerosols in a Laboratory Rotating Drum. SEAN KINAHAN, Don Collins, Yong-Le Pan, Aimable Kalume, Matthew Tezak, Keiko Salazar, Gabriel Lucero, Steven Storch, Cathryn Reyna, Joshua Santarpia, *Sandia National Laboratories*

A Goldberg rotating drum was established in a BSL-1 laboratory to age aerosols in the presence of controlled levels of relative humidity (RH), ozone, and UV light. More recently, a series of mass-flow controllers and permeation tubes were incorporated to achieve controlled, reproducible concentrations of volatile organic compounds (VOCs), with the focus to date on toluene and α-pinene. Gaseous species are continuously introduced along a center-axis using a gas-permeable expanded Teflon tube to maintain stable reaction conditions, while also maintaining a low velocity exchange of gases to prevent the disruption of the aerosol population. Three types of bioaerosols were produced to investigate the effects of these variables both individually, and with other input conditions expected to have combinatory effects. Specifically, a spore-forming species, Bacillus thuringiensis al Hakam, a vegetative species, E. coli, and a virus, MS-2, were grown according to established laboratory protocols and aerosolized through an ultrasonic nozzle at a particle size of 2-3 µm, depending on the organism. Changes in the bioaerosol population size and fluorescence were monitored using real-time aerosol instrumentation including a Wideband Integrated Bioaersosol Sensor (WIBS 4A), an Aerodynamic Particle Sizer (APS), and an Army Research Laboratory developed Single Particle Fluorescence Spectrometer (SPFS), which excites particles at both 263 and 351 nm wavelengths. Additionally, viability and genomic signature were investigated in aerosol samples collected using an AGI-30 impinger, allowing a comparison of an aged sample to the corresponding time zero sample. For Bacillus thuringiensis, UV light was found to be the primary driver of aging, with very minor effects of RH, ozone, and VOCs. Statistically significant increases in aging were observed for E. coli when exposed to UV light and toluene compared to UV light alone or toluene alone, despite UV light being the primary driver. Lastly, exposure to UV light and high RH resulted in increased aging in the presence of both VOCs for the virus, MS-2. In most cases, the magnitude of change in PCR signature did not correlate with the magnitude change in viability, even when the same overall trend was present, which also indicates differences in the decay of detectability and viability.

10BA.17

Spore Aerosol Viability Dependence on Radiation Exposure. MATTHEW B. HART, Jozsef Czege, Cathy S. Scotto, Jana Kesavan, Vipin Rastogi, Frank Handler, Jay D. Eversole, *Naval Research Laboratory*

We report results from our study in which two types of *Bacillus* spores were prepared and aerosolized into a linear electrodynamic quadrupole (LEQ) trap for the purpose of exposing them to ultraviolet (UV) light sources to determine loss of viability as a function of exposure (time) based on subsequent collection, plating and counting. As part of a DTRA JSTO funded collaboration, *Bacillus thuringiensis* Al Hakam and *B. anthracis* Sterne samples were prepared as phase-bright spores, multiply washed and resuspended in pure water with 0.01% polysorbate 80. Spore samples were titered at the beginning of each experiment, and 70 µm diameter suspension microdroplets were generated using a piezo-electric transducer coupled to a quartz capillary nozzle.

The LEQ was aligned with its symmetry axis vertical, and the nozzle tip was positioned at the top of the trap pointing down along the central axis. Microdroplets were inductively charged as they were ejected into the LEQ. The LEQ was partitioned into upper and lower chambers. Typically, several hundred to a thousand droplets were initially produced and confined in the upper chamber. Drying occurred in seconds, and the spores in each microdroplet (with some fraction of surfactant residue) formed a single particle (spore cluster). Since droplets were generated with a fixed uniform size, the number of spores in each particle was proportional to the spore suspension concentration. The distribution of spores per particle (particle size distribution) is governed by Poisson statistical variability of the number of spores in a 70 µm diameter droplet of suspension fluid. For example, a concentration of 1.25 x 10^8 spores/ml yields a mean number of 22 spores per droplet, with a standard deviation of +/-4.7 (corresponding to ≈ 3.3 +/-0.2 µm diameter clusters when dried).

The LEQ consists of four 120 mm long, 1.5 mm diameter electrodes arranged on a square with 8.0 mm sides. An airtight enclosure for this system was fabricated with windows for optical exposure and interrogation. The LEQ was partitioned into upper and lower chambers by two concentric conductive rings perpendicular to the electrodes, and centered on the symmetry axis. These rings were held at a fixed potential with the same polarity as the particles, and functioned as an electrical valve holding the charged particles in the upper portion of the LEQ during exposure. After exposure, trapped particles could flow from the top chamber to the lower chamber by decreasing the ring potential. A second pair of rings was positioned at the bottom of the lower chamber to hold particles there for image-based counting prior to flowing them through a membrane filter for collection as they exit the enclosure.

The radiation exposure study uses both a solar simulator (Oriel model 94021A), and a low-pressure Hg discharge lamp (>94% intensity @ 254 nm). Both the spectrum and the intensity of these lamps are periodically monitored to ensure continuity for a fixed output. We are currently scoping exposure times for two or three sample concentrations as described above. This initial study will bracket “short” and “long” exposure times (with no-exposure controls with the same times) to select an appropriate exposure range to obtain meaningful decay rate data. We will present our latest results for both spore species generated as “single” spore particles and also as larger spore clusters, for both the 254 nm (UV-C) lamp and the solar simulator.

10BA.18

Spatial and Longitudinal Influences on Accurately Predicting a Microbiome “Biofingerprint”. ANDREW HOISINGTON, Christopher Stamper, Katherine Bates, Christopher Lowry, *Air Force Institute of Technology*

Indoor bacterial communities have been linked to the human occupants. More specifically, the human skin bacterial microbial communities have been observed to influence the bacteria identified on surfaces (Hewitt et al., 2012; Dunn et al., 2013) , likely from the contact of the surfaces with hands. Humans share in common only approximately 10% of their skin microbes (Gonzales et al., 2014), which might provide a unique marker for each individual who has touched a surface as well as a way to model the passage of bacteria from person to person via a fomite. Lax et al. (2014) found in a longitudinal study of residential microbes that humans sharing the same home had the most similar microbial skin communities, and that the skin microbial communities of individuals could be used to accurately predict the individual’s home. This study was conducted in two separate locations; work and home environments. Samples were collected once a week for the three consecutive weeks at both locations from the human and built environmental microbiomes. Bacterial DNA was extracted from the samples, amplified, and sequenced on an Illumina MiSeq platform. Bacterial communities were characterized and supervised learning models were used to determine if samples are associated with the participants. Further supervised learning models were used to determine the predictive power for associating possessions and spaces to the owner/ occupant. Finally, supervised learning models and LEfSe analysis were used to determine specific taxa that are biomarkers of the gender associated with a sample. We determined that supervised learning models can associate a participant with their possessions and spaces with a high degree of certainty (90% and 94% accurate for work and home environments, respectively). We also determined that there are varying levels of predictive power associated with the different sample types in determining the identity of the owner/ occupant. In general surfaces commonly in contact with the hand (i.e. computer mouse and computer keyboard) were very good at training supervised learning models to predict the owner/ occupant (~73% accurate). While samples that rarely come in direct contact with the hand (i.e., bedroom floor) were not very good at training supervised learning models to predict the owner/ occupant (~13% accurate). We were able to show that, over the three-week sampling period, sample types had relatively stable bacterial communities, and that some sample types are more longitudinally stable than others. For instance, the computer mouse was highly stable longitudinally, while the hand is more variable. Overall, this study showed that bacterial communities can be used to accurately associate items and spaces to a specific owner/ occupant with a high degree of certainty. Effectively adding to the growing body of evidence that individuals leave a microbial “biofingerprint” on items they touch and spaces they occupy.

10BA.20

Aerosolization of Biological Aerosols: Principles and Pitfalls. GEDIMINAS MAINELIS, Huajun Zhen, Taewon Han, *Rutgers, The State University of New Jersey*

Bioaerosol generation is an important aspect of bioaerosol research, and reliable and robust methods are needed to produce steady bioaerosol streams of desired concentrations with minimum damage or other negative effects to the aerosolized biological particles.

This presentation will focus on liquid-based bioaerosol generation techniques and will explore the main principles of commonly used devices, such as various atomizers and bubbling-based bioaerosol. The talk will then explore pitfalls of bioaerosol generation, namely potential damage to bacterial and fungal cells and various options for minimizing such damage. As a case in point, the effect on culturability and membrane integrity *Escherichia coli* when aerosolized by four different devices will be explored. Here, Collison nebulizer, a Liquid-Sparging Aerosolizer (LSA), a C-flow nebulizer, and a recently-designed Single-Pass Aerosolizer (SPA), which is a single-pass pneumatic nebulizer, aerosolized *E. coli* under different device regimes.

The extent of cell membrane damage was determined as the Cell Membrane Damage Index, which was expressed as the ratio of cell-released 16S rRNA gene copies in sample liquid versus the entire amount of 16S rRNA gene copies in a bioaerosol sample. The Damage Indices for *E. coli* aerosolized with the Collison and C-flow nebulizers at 40 psi were significantly higher than the corresponding Indices at nebulization pressures of 5 and 15 psi. However, the increased aerosolization pressure for LSA and SPA did not have a substantial impact on cell membrane damage. Collison nebulizer and SPA were observed to cause increased culturability loss with increased aerosolization pressure (5 to 15 psi for Collision nebulizer and 5 to 40 psi for SPA), while the other two generators did not increase the loss of culturability with increased aerosolization pressure. At a constant aerosol concentration of 100 bacteria/cm^3, the SPA showed the highest bacterial culturability among the tested generators. Only the Collison nebulizer and SPA achieved aerosol concentrations of 1000 bacteria/cm^3, and the SPA outperformed the Collison nebulizer with respect to cell membrane damage. In another aspect of this investigation, a fraction of particles <0.523 µm, i.e., fragments of bacteria, increased for all devices with increasing aerosolization pressure. Overall, the results demonstrate that the extent of cell damage due to aerosolization could be managed by selecting different aerosolization techniques and by carefully choosing operational parameters of those techniques.

10BA.21

Surgical Smoke: A Literature Review. CATHERINE ALMQUIST, *Miami University*

Surgical smokes are generated in the operating room when surgeons remove tissue with laser treatments. The surgical smokes are known hazards to operating room personnel, as they may contain viruses, bacteria, and carcinogens, among other known hazards.

This poster is a review of surgical smokes: What are they? How are they formed? What are the risks? How are they mitigated? What are the future needs to reduce the hazards of surgical smokes?

10BA.23

Bioaerosol Characterisation in the Transportation Environment. IAN COLBECK, Nikoletta Grydaki, Corinne Whitby,
University of Essex, Colchester, CO4 3SQ, UK

Scientific studies have shown that commuting results in significant contribution to the daily exposure to air pollutants, which is highly affected by the mode of transport. Recently, the microbial fraction of particles has started receiving attention and a number studies have been conducted covering various means of transport. Moreover, findings reported in literature are mainly based on culture-based method. The aim of the current study was to investigate the abundance and diversity of the airborne micro-organisms in cars and trains on a commuter route. Air samples were collected and airborne bacteria characterised by high-throughput sequencing of 16S rRNA.

Bacterial levels during commuting by train ranged from 5.8×10^4 to 9.4×10^4 *E. coli* genome equivalents/m^3 during morning, from 4.4×10^4 to 7.9×10^4 *E.* genome equivalents/m^3 during afternoon and from 9.4×10^4 to 1.3×10^5 genome equivalents/m^3 during evening journeys When comparing the two types of transport mode independent samples t-test confirmed that bacterial levels were significantly greater in train journeys compared to car journeys (p-value = $0.019 < 0.05$).

At the class level, *Actinobacteria* showed the highest relative abundance across all train samples followed by *Gammaproteobacteria*. For the car samples, the most abundant bacterial classes on average were *Bacilli* and *Actinobacteria*. At the genus level human-skin associated genera including *Corynebacterium* and *Staphylococcus* were present in both trains and cars.

In summary the bacteria that were found in varying abundances in the air of the microenvironments belonged to the human-associated *Corynebacterium* spp. (2 OTUs), *Streptococcus* spp., *Staphylococcus* spp. (2 OTUs) and outdoor environment-related taxa *Blastococcus, Brachybacterium, Hymenobacter, Arthrobacter* and *Carnobacterium*.

10BA.24

Optimize Aerosolized Generation and Characterization of Bacterial Spores. KAVINDRA KUMARAGAMA, Jing Qian, Shane Rogers, Shantanu Sur, Suresh Dhaniyala, *Clarkson University, Potsdam, NY, USA*

Airborne particles, particularly those smaller than 2.5 µm, can cause adverse health effects. The health impact of exposure to particles can be magnified when the particles are biological in nature. As an example, exposure to *Bacillus anthracis (Ba)* can result in death, thus, knowledge of *Ba* transport characteristics and fate in the environment is critical. *Bacillus* species form highly resistant endospores that remain viable in the environment for many years until contact with favorable environmental conditions, and they can disseminate through aerosolization. Here, we have developed and tested methods to generate and characterize a surrogate for *Ba*, *Bacillus thuringiensis*. In our tests, we cultured and purified spores (>90% purity) in a BSL-2 facility, and used nebulization to aerosolize them. In the first step, we optimized the purification process by characterizing the relative distributions of spores and cells in the different steps of the process. We explored the aerosolized particle characteristics under different spore suspension concentrations. Under low concentrations of the suspension, the mean aerodynamic diameter of single *Bacillus thuringiensis* spores was 0.72 µm. At higher concentrations of the suspensions, spore clusters with aerodynamic diameters as large as 2 µm were observed. Spore and spore cluster sizes were confirmed with Six-stage Viable Andersen cascade impactor-based measurements. Spore viability during nebulization and deposition was investigated using fluorescent stains acridine orange (all cells) and propidium iodide (permeabilized cells). The validated spore generation process is being used in experiments to deposit single spores and clusters of different sizes on substrates. The objective is to determine forces required to remove these biological particles from substrates of different compositions.

10BA.25

Variability of PM and Bioaerosols at Diverse Indoor and Outdoor Locations in a Southern Tropical Indian Region.

HEMA PRIYAMVADA, Priyanka C., Raj Kamal Singh, Akila M., Ravikrishna R., Sachin S. Gunthe, *Clarkson University*

This study discusses the relationship and variations in the indoor-outdoor PM concentrations, size-resolved bioaerosol concentration, size distribution and diversity, I/O ratios of PM and bioaerosol, indoor bioaerosol emissions for five diverse yet commonly encountered locations. The $PM_{2.5}$ and PM_{10} concentration trends were similar across all the indoor and outdoor locations investigated. Highest PM concentrations observed at the eatery was due to the elevated cooking activity and human movement induced floor resuspensions. The I/O mass concentration ratios of PM revealed a notable influence of outdoor PM in the indoor environment of laboratory. Variations in PM concentrations at indoor and outdoor environments were substantiated with ANOVA and chi-square p-values. Human occupancy also contributed to higher bioaerosol concentrations (>800 CFU m^{-3}) in the indoor. The indoor-outdoor fungal aerosols concentration trends were similar across all locations. Fine to coarse bioaerosol fractions indicated an abundant presence of coarse mode bacteria and fungi amounting to >80% of the total cultivable bioaerosol load in all locations. DNA analysis revealed *Bacilli* and *Gammaproteobacteria* to dominate the bacterial aerosols while *Cladosporium* and *Aspergillus* dominated the fungal aerosols. Fungi contributed highest to the mass fraction of PM_{10} in comparison to bacteria, both indoor and outdoor. Highest bacterial emission rates were observed at air-conditioned room (4.85×10^5 CFU/h/person) and fungal emissions at the laboratory (4.60×10^5 CFU/h/person). Very few such studies of public health importance are available over Indian region with almost none, simultaneously investigating PM and bioaerosols of indoors over southern India.

Keywords: indoor; PM; bioaerosols; I/O ratio; size distribution; emission rates

10CA.1

A Differential Photoacoustic Spectroscopic (DPAS) Technique for Aerosol Light Absorption Measurement in the Presence of Light-absorbing Gaseous Species. ZHENHONG YU, Gregory Magoon, William Brown, James Assif, Richard Miake-Lye, David Liscinsky, *Aerodyne Research, Inc.*

We developed a differential photoacoustic absorption spectroscopic (DPAS) technique to measure light absorption from particulate matter (PM) at the spectral region from 360nm to 1064nm, in the presence of light-absorbing gaseous species. It is capable of operating in a single-wavelength or multiple-wavelength configuration. The dual-cell DPAS system contains two identical single-pass photoacoustic cells to measure the photoacoustic signals due to light absorption of total PM + gaseous samples and that of gaseous samples alone, separately. The precise dimension and single-pass configuration of the photoacoustic cells guarantee that optical path length, resonance frequency, cavity quality of the two cells are virtually identical. The resulting differential photoacoustic signal can be used to determine the light absorption purely from the PM species. This measurement method eliminates the interferences from the light-absorbing gaseous species as well as the surrounding low-frequency background acoustic noises.

A high-power continuous-wave diode-pumped solid state (DPSS) laser with good beam quality at 532nm was used as the light source of the DPAS system. The laser output was amplitude modulated at the resonance frequency of the photoacoustic cells via a waveform control on its electrical DC power supply. Given the small dimension of the silicon-based microelectromechanical system (MEMS) microphone, we found that a linear-array detector with multiple microphones can be applied as the photoacoustic detector, which doubles the S/N relative to a single microphone detector.

Photoacoustic signals of the DPAS monitor at 532nm were calibrated with NO_2 gas standards. Based on an Allan analysis, a detection sensitivity (2δ) of 0.30 Mm-1 can be achieved in 100s data acquisition at 532nm.

Using the Jet Burner Test Stand (JBTS) facility at the United Technologies Research Center (UTRC), we measured light absorption by the aviation soot emissions from a representative high-temperature and high-pressure test combustor for aircraft auxiliary power units (APU). The DPAS measurement results at 532nm, under the high gaseous NO_2 conditions, were then compared to the determination of soot mass concentrations from an AVL Micro Soot Sensor (MSS). An excellent linear correlation between the measurements from two instruments was observed. The mass absorption coefficient (MAC) of the aviation soot was determined to be $7.4 \pm 0.1\ m^2\ g^{-1}$, in good agreement with the expected value of $7.6 \pm 0.6\ m^2\ g^{-1}$.

10CA.2

Laboratory-Generated Coated Soot Aerosols with Tunable Physical, Chemical and Optical Properties Using a Cast Generator and a Portable Micro Smog Chamber. Michaela N. Ess, Alejandro Keller, Adam Kimak, Heinz Burtscher, KONSTANTINA VASILATOU, *METAS*

Particles in ambient air usually consist of a solid fraction, such as elemental carbon or minerals, and a more or less volatile fraction. Depending on temperature and volatility, this fraction may condense on the surface of preexisting particles, remain in the gas phase or nucleate and form new particles. This is strongly influenced by chemical reactions occurring in the atmosphere (mainly atmospheric oxidation known as aging) that lead to the formation of secondary organic aerosol (SOA; i.e. organic matter formed from organic gaseous precursors which -upon atmospheric oxidation- condense on preexisting particles or nucleate to form new particles).

In our study, we show that coated soot particles mimicking the properties of aged carbonaceous aerosols in the atmosphere can be synthesized in the laboratory. The soot core particles were generated with a CAST burner and subsequently mixed with vapors of a preselected gaseous precursor in a photo-oxidation reactor (Micro Smog Chamber, [1]). Experiments were performed with precursors of both biogenic and anthropogenic origin, such as α-pinene and 1,3,5-trimethylbenzene (TMB), respectively.

The Micro Smog Chamber has been used in the past to simulate the SOA formation potential of wood stove emissions [2,3] and has been compared to other common tools aiming to simulate atmospheric aging in the lab, including large-scale smog chambers [4]. It has been shown that MSC generates SOA of realistic chemical composition with yields within the range expected from previous smog-chamber studies. Compared to smog chambers the MSC offers the following advantages:
i) the device is compact, portable and easy to use;
ii) the generation of SOA and coating of particles is much faster due to the small size of the reactor and the high power of the UV radiation.

We have found that with MSC combustion particles can be coated with organic matter of biogenic/anthropogenic origin in a matter of seconds. As example, for 200 nm soot particles the thickness of the coating can be easily varied between a few nm to about 150 nm. Upon coating, the fractal-like structure of fresh soot collapses to give more compact soot core particles, a process known to occur often in the atmosphere. Moreover, the EC/OC ratio of the coated particles can be readily adjusted between 98:2 and 20:80. Measurements are under way in order to determine the optical properties of the coated particles, such as the absorption coefficient and single scattering albedo (SSA).

Thanks to their controlled and tunable properties these lab-generated carbonaceous aerosols have the potential to serve as reference aerosols to challenge common field instruments measuring equivalent Black carbon (EBC), such as aethalometers. These filter-based instruments suffer from complex measuring artefacts and high measurement uncertainties. Joint efforts are undertaken within the EMPIR-Black Carbon European research project to develop a validated method for their calibration [5].

Moreover, the stable and reproducible generation of coated carbonaceous aerosols in the lab is the first step towards more complex synthetic ambient aerosols as described in the EMPIR-Aeromet project [6].

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10CA.3

The Density, Morphology, and Internal Structure of Biomass Burning Brown Carbon Aerosol. BENJAMIN SUMLIN, Christopher Oxford, Bongjin Seo, Robert Pattison, Brent Williams, Rajan K. Chakrabarty, *Washington University in St. Louis*

Recent studies have reported the ubiquitous presence of brown carbon (BrC) aerosol in the atmosphere. These particles, predominantly emitted from biomass burning, strongly absorb light in the near-ultraviolet wavelengths and offset the radiative cooling effects associated with organic aerosols. The density of a particle is an important physical property of aerosols, because it determines the transport of particles in the atmosphere and the human respiratory system, as well as their optical properties such as refractive index, which tends to increase with increasing density [1].

Our current knowledge of this particle property is limited, especially when considering the influence of combustion temperature and fuel type. For non-spherical or inhomogeneous particles, the dynamic shape factor must be included when relating the aerodynamic and mobility diameters. This dimensionless parameter accounts for the effect of non-sphericity on the particle drag force. It is difficult to accurately determine the dynamic shape factor for a single particle. With the advent of mass-based classifiers, an alternative particle property, the effective density (ρ_{eff}), has recently been adopted by the atmospheric aerosol community [2-4].

We measured ρ_{eff} of primary BrC aerosol emitted from smoldering combustion of Boreal peatlands using a differential mobility analyzer, a centrifugal particle mass analyzer, and a condensation particle counter. We controlled energy transfer into the fuel by altering the combustion ignition temperature, and we find that the particle ρeff ranged from 0.85 to 1.19 g cm^{-3} with ignition temperatures from 180 to 360 °C. Spherical morphology was observed from electron microscopy analysis, and the mass–mobility exponent was a constant 3.0, indicating no internal microstructure or void spaces. Additionally, variation in ρ_{eff} upon partial volatilization by a volatility tandem differential mobility analyzer was analyzed to study the properties of the organic matter constituting these particles. The ρ_{eff} of particle phase mass remaining after thermal volatilization was confined to a narrow range between 0.9 and 1.1 g cm^{-3}. These findings lead us to conclude that primary BrC aerosols from biomass burning have homogeneous internal composition, and their ρ_{eff} is in fact their actual density.

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10CA.5

The Effect of Potassium Chloride Addition on the Characteristics of Nascent Soot during Ethylene Pyrolysis. Mengda Wang, JUNYU MEI, Quanxi Tang, Xiaoqing You, *Tsinghua University*

Soot as incomplete combustion products has been studied extensively due to its detrimental effect on the environment and human health. For combustion of solid fuel, such as coals and biomass, abundant alkaline and alkaline earth metals would have an interaction with the formation of soot particles. Besides, inorganic substances containing potassium were widely used as additives to improve the quality of carbon black generated from the industrial production process.

In this work, the effect of KCl addition on the characteristics of soot particles formed during the pyrolysis of ethylene/water/nitrogen flow in a flow reactor has been investigated. Particle size distribution functions (PSDFs) of soot particles formed in the flow reactor at different residence time were measured by using micro-orifice probe sampling in tandem with scan mobility particle sizer (SMPS). Meanwhile, a differential mobility analyzer (DMA) applied with a fixed voltage in tandem with SMPS was used to explore the charge characteristics of soot particles. In addition, the morphology of soot particles sampled from the probe was examined using transmission electron microscopy (TEM). From the PSDFs, it was observed that the addition of KCl did not affect much the nucleation of soot particles, but inhibited the growth of soot particles. Besides, the number of particles with double positive charges decreases with the addition of KCl, which indicates the KCl addition neutralized the multi-charged particles. Consequently, the coagulation rate between soot particles was reduced, which led to smaller particles and slower growth by coagulation. Compared to the results of the reference mixture without KCl addition, in the KCl-added mixtures, both the TEM images and the mass-mobility exponent show that soot particles are generally more compact, and the primary particles of soot aggregates have a narrower size distribution and a smaller median diameter.

10CA.6

Spectral Measurements of Mass Absorption Cross-Section of Flare-Generated Black Carbon. BRADLEY CONRAD, Melina Jefferson, Brian Crosland, Matthew Johnson, *Carleton University*

Gas flaring is a ubiquitous process in the upstream oil and gas industry where unwanted gaseous product is destroyed through open-to-atmosphere combustion. Flaring is a significant global source of atmospheric black carbon (BC), a pollutant second only to carbon dioxide in terms of radiative climate forcing (Jacobson 2001). With respect to the climate, the crucial property relating the mass of BC to its radiative forcing potential is the mass-normalized absorption cross-section (MAC, in units of area per mass). Additionally, MAC is also a necessary variable in optical diagnostics that quantify BC mass from observed attenuation of light. In their well-cited review, Bond & Bergstrom (2006) suggest that a fixed value of MAC should exist for all combustion-generated BC, especially with respect to notable uncertainties in its measurement. The authors also note however, that absorption by BC is sensitive to the degree of graphitization of BC particles, which occurs at elevated temperatures as particles traverse the length of the flame. This inherently suggests a dependence of MAC on the time-temperature history of flame-generated BC. Since buoyancy-driven gas flares are generally much larger in scale than other important combustion-generated BC sources, such as diesel and spark-ignition engines, this notion suggests that the MAC of flare-generated BC (and other sources for that matter) could indeed be different than the value presented by Bond & Bergstrom (2006).

This work presents spectral measurements of MAC of fresh flare-generated BC on laboratory-scale flares representative of the upstream oil and gas industry. Experiments of flares of up to approximately 8' in length are performed at the Carleton University Flare Facility in Ottawa, Canada via vertically-oriented flare stacks spanning 1.5" to 3" in diameter. Combusted flare gas compositions of up to nine components representative of measured flare gases in Alberta, North Dakota, Ecuador, the North Sea, and Russia are combusted over a range of volumetric flow rates. Absorption data from a three-wavelength photoacoustic soot spectrometer (Droplet Measurement Technologies) spanning the visible spectrum is coupled with carbon mass data from a semi-continuous, thermal/optical organic carbon-elemental carbon analyzer (Sunset Laboratory) to directly quantify flare-generated BC MAC. In this study, the focus is to assess the sensitivity of BC MAC to various flare conditions. To this end, fuel flow rates are selected to enable the isolated assessment of BC MAC as a function of flare aerodynamic parameters (e.g. Reynolds number, Froude number, and flame length) in addition to chemical properties defined by flare gas composition.

10CA.7

Temperature Effects on Carbonaceous Particle Formation during Ethylene Pyrolysis in a Laminar Flow Reactor. JUNYU MEI, Mengda Wang, Xiaoqing You, Chung K. Law, *Tsinghua University*

Evolution of the particle size distribution functions (PSDFs) during ethylene pyrolysis in the laminar flow reactor was measured by a scanning mobility particle sizer coupled with the small orifice sampling technique. The sampling dilution ratio was calibrated and determined to eliminate the effects of particle loss in the sampling line. Investigation of various possible effects on the PSDFs indicates that while the PSDFs are very sensitive to the inlet flow rate, they are not much affected by the probe location and the sampling delay time within operating errors. Evolution of the PSDFs is realized by varying the inlet flow rates and compared for different ethylene concentrations (0.4%, 0.6%, 0.8%) and tube temperatures (1573K, 1673K, 1773K). A distinct bimodal distribution is observed in all pyrolysis cases. The particle size distribution is found to be very sensitive to both temperature and fuel concentration. The increase of temperature leads to an exponential decrease of induction time for particle formation. The higher the fuel concentration, the earlier the soot inception occurs and the faster are the soot nucleation and mass growth rates.

10CA.8

Use of Electron Tomography to Analyze the Actual Primary Particles Distribution and Agglomerate Morphology of Soot. Alberto Baldelli, STEVEN ROGAK, Una Trivanovic, *University of British Columbia*

Measuring the properties of soot agglomerates is fundamental to the understanding of their impact to the prediction of emission rates and of climate forcing of black carbon particles. Here, soot samples were collected from a large lab-scale flare of up to 80 mm in diameter with turbulent flames up to 3 m tall. The flare initial conditions vary in fuel composition, a mixture of methane, ethane, propane, butane, N2, and CO2, according to the burner diameters, 38, 51, and 76 mm. The flare exit velocity ranged from 0.5 to 1.5 m/s.

A previous literature reference showed that imaging soot agglomerates in 3D, with an electron tomography, can help to understand their complex morphology to observe details that are challenging to be determined when analyzing them in 2D. One of the findings from the 3D tomography is that soot agglomerates exhibit ring structures, in contrast to expectations from classical, perfect-sticking Cluster-Cluster Aggregation models.

The electron tomography of soot agglomerates consists of a group of 2D images taken each 2° in a range of view that goes from -70 to 70°. This study aims to use a validated code, designed for the analysis of 2D images, with the results obtained with electron tomography to determine the primary particle size distribution. Thus, the dependence of the primary particle distribution and the projected angle of the soot agglomerate is estimated.

10CA.10
Quantitative Comparison of Correction Algorithms Applied Filter-Based Black Carbon Measurements during the FIREX Campaign. HANYANG LI, Gavin McMeeking, Andrew May, *The Ohio State University*

Light absorption by black carbon (BC) particles in the atmosphere is predominantly measured using filter-based techniques. In these instruments, light is transmitted through a filter; changes in transmission are quantified as "attenuation", which is then related to light absorption. However, measured light attenuation may be overestimated or underestimated due to filter-loading artifact during sampling and light scattering artifact by filter fibers and embedded aerosols. Consequently, several correction algorithms (derived based on ambient aerosols where the concentration was roughly constant) have been introduced to minimize such artifacts. Moreover, to convert absorption to mass concentration, a mass absorption coefficient (MAC) is required. Hence, another uncertainty associated with the quantification of filter-based BC is the selection of an appropriate MAC. While it is widely accepted that applying correction algorithms and site-specific MACs improve the agreement among different filter-based BC instruments, it is uncertain whether any correction algorithm and MAC can be regarded as 'benchmarks' as both factors may depend on properties of aerosols and BC concentrations. These uncertainties may be even larger for biomass burning aerosols, which are inherently different (chemically and optically) than most typical ambient aerosols.

Experiments were conducted during 2016 FIREX Campaign to investigate BC emissions from simulated wildfires in the laboratory including three filter-based absorption measurements: a 7-wavelength aethalometer (Aeth-7), a Continuous Light Absorption Photometer (CLAP), and a Tricolor Absorption Photometer (TAP). In this presentation, we will summarize MACs of filter-based absorption measurements during the Campaign and quantitatively compare four published Aeth-7 correction algorithms and two Particle/Soot Absorption Photometers (PSAP) corrections (applicable to CLAP and TAP). While evaluations of correction schemes have been conducted in the past, none have focused on biomass burning smoke (and none have systematically compared schemes applied to CLAP and TAP); thus, our dataset allows us to explore how well these correction algorithms compare to a reference in situ light absorption measurement (a Droplet Measurement Techniques (DMT) Photoacoustic Extintiometer (PAX)).

Our analysis indicates that MAC strongly depends on aerosol properties. For example, an increase in MAC is observed due to the presence of brown carbon. Furthermore, filter-loading and light scattering artifacts can be clearly identified after a filter spot change, especially during fires with low single scattering albedo (relative to the atmosphere). Finally, applying correction algorithms results in high correlations between instruments. Although we cannot be certain that any correction algorithm gives us an unequivocally correct value, we will assess the degree of agreement between different algorithms, accounting for differences in chemical and optical properties. We are continuing to explore the role of the aerosol optical properties of biomass burning on differences among correction algorithms in order to provide a robust set of recommendations that can be used to constrain the uncertainty of filter-based BC measurement techniques and improve emission inventory of BC emission factors.

10CA.11

Influence of Aging on Mass Absorption Coefficient and Single Scattering Albedo of SOA: Oxidation vs. Organo-nitrate Formation. STEPHEN ZIMMERMAN, Justin Dingle, Alexander Frie, Justin Min, Roya Bahreini, *University of California, Riverside*

Atmospheric particles directly influence the global radiative budget by absorbing and scattering solar radiation. In this study, chemical and microphysical properties of secondary organic aerosol (SOA) generated in a smog chamber are tracked to investigate effects of aging on SOA mass absorption coefficient (MAC) and single scattering albedo (SSA). SOA is formed via photooxidation of biogenic (α-pinene [AP] and longifolene [LGF]), and aromatic (1-methylnaphthalene [1-MN], Phenol [PH], and Toluene [TOL]) compounds with hydroxyl radical ($OH^{\cdot}$) in the presence of low and high concentrations of nitrogen oxides (NO_x), using hydrogen peroxide (H_2O_2) and HONO as the $OH^{\cdot}$ source. An Aerodyne mini-aerosol mass spectrometer (mAMS) is used to obtain fast, size-resolved, non-refractory chemical composition and mass concentrations of organic and nitrate submicron particles while online optical properties are measured by a Cavity Attenuated Phase-Shift (CAPS, at 632 nm) spectrometer and Photoacoustic Extinctiometer (PAX, at 375 nm). Fractional contribution of CO_2^+ from organic aerosol, ratios of $C_2H_3O^+/CO_2^+$, and average carbon oxidation states (OSc) are calculated to capture the effect of aging on the bulk aerosol as oxidation occurs. Additionally, contributions of organo-nitrates are estimated by comparing the observed NO^+/NO_2^+ ratios of SOA with that of known organo-nitrate compounds and NH_4NO_3. Lower NO^+/NO_2^+ ratio values (2-5) are observed from H_2O_2-sourced $OH^{\cdot}$ while ratios from HONO-sourced $OH^{\cdot}$ range from 3-8, suggesting formation of more organo-nitrates with HONO. During HONO experiments, the NO^+/NO_2^+ ratios are highest at the beginning of the SOA growth and decrease as oxidation proceeds. On the other hand, MAC increases monotonously with oxidation; such observations suggest chromophores other than organo-nitrates are being formed that contribute to the increase in relative absorption. MAC values calculated at 375 nm have similar ranges from 0.01-4 (m^2/g) when comparing between oxidant sources. Biogenic SOA have smaller maximum MAC values ≈0.3 (m^2/g) than aromatic SOA, which have a range of maximums, from 1-4 (m^2/g) depending on the precursor VOC. Further investigation will be conducted to identify the major chemical components driving the observed changes in optical properties.

10CA.12

UV-Vis-IR Spectral Complex Refractive Indices and Optical Properties of Brown Carbon Aerosol from Biomass Burning.

YULI W. HEINSON, Benjamin Sumlin, Nishit Shetty, Apoorva Pandey, Brent Williams, Rajan K. Chakrabarty, *Washington University in Saint Louis*

BrC aerosols have a significant uncertainty on radiative forcing and climate models. Constraining the complex refractive indices, optical properties and size of brown carbon (BrC) aerosols is a vital endeavor for improving climate models and satellite retrieval algorithms. Smoldering peatlands have been identified as a major emission source of these aerosol. The fuel parameters such as moisture content, source depth, geographic origin, and fuel packing density of the wildland fuels could influence the properties of emitted aerosol. We measured in situ spectral (375-1047 nm) optical properties of BrC aerosols emitted from smoldering combustion of Boreal and Indonesian peatlands across a range of the fuel parameters. Inverse Lorenz-Mie algorithms used these optical measurements along with simultaneously measured particle size distributions to retrieve the aerosol complex refractive indices ($m=n+i\kappa$). Our results show that the real part n is constrained between 1.5 and 1.7 with no obvious functionality in wavelength (λ), moisture content, source depth, or fuel packing density (FPD). With increasing λ from 375 to 532 nm, κ decreased from 0.014 to 0.003 following the Kramers-Kronig dispersion relation for the damped simple harmonic oscillator, with a corresponding increase in single scattering albedo (SSA) from 0.93 to 0.99. For $\lambda \geq 532$ nm, both κ and SSA show no spectral dependency.

10CA.13

Fractal Morphology of Black Carbon Aerosol Enhances Absorption on the Thermal Infrared Wavelengths. WILLIAM HEINSON, Rajan K. Chakrabarty, *Washington University in St. Louis*

We numerically calculate the mass absorption cross sections (MACs) of black carbon fractal aggregates in the thermal infrared solar spectrum. Compared to equivalent-size spheres, the MAC values of aggregates show a percent enhancement of ≈150 and 400 at small and large length scales, respectively. The absorption properties of aggregates with size parameters >1 surprisingly continued to remain in the Rayleigh optics regime. We explain this phenomenon using the Maxwell–Garnett effective medium theory and the concept of phase shift parameter.

10CA.14

A New Method for the Determination of BC Mass Concentration from Light Absorption. YINGLI YU, Chunsheng Zhao, Wangshu Tan, *Peking University*

Atmospheric black carbon (BC) is the strongest visible solar radiative absorber in the atmosphere, exerting significant influences on the earth's radiation budget. The mass absorption cross-section (MAC), describing the light absorption ability per unit mass, is a crucial parameter for the conversion of light absorption coefficient to mass equivalent BC concentrations. MAC is influenced by many factors such as aerosol mixing state, BC core size and aerosol refractive index. However, MAC is a constant for the filter-based measurements to calculate BC mass concentration, introducing significant uncertainties. In this paper, we develop a look-up table of MAC, BC core size and particle size. An iterative algorithm for the conversion of light absorption coefficient to BC mass concentration is proposed by considering the influences of BC mixing state and BC core size on MAC. The results show that AE33(widely used filter-based instrument) underestimates the BC mass loading by 35% for aerosol particles smaller than 270nm and overestimates the BC mass loading by 20% for aerosol particles larger than 270nm. This work deepens our understanding in the influences of mixing state on BC optical properties and is helpful for the uncertainty constraining of BC mass concentration measurements.

10CA.15

Effects of Thermodenuding on the Morphology and Optical Properties of Soot. NISHIT SHETTY, Apoorva Pandey, Yuli W. Heinson, Rajan K. Chakrabarty, *Washington University in St. Louis*

Soot particles are composed of refractory elemental carbon and have varying amounts of condensed organic carbon coating. The optical properties of soot depend on the complex refractive indices and the effective size of the coated particles, as well as the particle morphology. A preferred methodology to investigate the change in optical properties of soot due to coating is to perform experiments with and without a thermodenuder. The conventional view is that the particle morphology doesn't change upon thermodenuding; we investigate the validity of this assumption in this study.

We performed experiments to investigate the effect of coating on the optical properties of soot generated from biomass burning and kerosene lamp. The organic coating was removed using a thermodenuder (Brechtel inc.) and the resulting change in absorption and scattering coefficients was measured using an integrated photoacoustic-nephelometer. In a separate set of experiments, the aerosol was passed through an angle-resolved static light scattering apparatus which provides information on the morphology of particles using q-space analysis of the scattered light. We monitored the change in soot morphology as a function of burn parameters using this optical setup. This poster will outline our findings from these set of experiments.

10CB.1

Investigating the Effect of Varying Ethanol Content and Driving Conditions on FFV-GDI Vehicle Emissions with the Addition of an Anthropogenic Surrogate. PATRICK ROTH, Jiacheng Yang, Ayla Moretti, Thomas D. Durbin, David R. Cocker III, Georgios Karavalakis, Akua Asa-Awuku, *University of California, Riverside*

GDI technology has become the preferred standard to PFI engines in the US and European markets due to its increased specific output and improved fuel economy. GDI vehicles have displayed increased PM emissions, meaning manufacturers of GDI engines may have difficulty meeting the new two phase LEV III PM Standard set at 3 mg/mile by 2017, and 1 mg/mile by 2025. One measure to meet the strict PM emissions standards is utilizing alternative fuel formulations (i.e., high ethanol blends). Currently commercial gasoline blends contain 10% ethanol but previous vehicle studies evaluating the effects of additional ethanol in fuels have found reductions in PM formation, however, the secondary aerosol formation is not understood.

Many previous studies have explored the secondary formation from vehicle exhaust in a clean chamber environment, however, simulating a dirtier urban environment is much more difficult. To execute this, an anthropogenic reactive organic gas (ROG) surrogate was designed to mimic the LA Basin. Emissions data was lumped into categories, and in each category species were weighted by abundance. The surrogate was designed to provide a base chemical reactivity while forming a minimal amount of SOA mass. The surrogate has been utilized in many previous studies at UCR, exploring ozone incremental reacting and SOA formation from single compound experiments, however this is the first study using the surrogate with a complex vehicle exhaust mixture. The goal of the surrogate mixture is to control the gas-phase chemical environment within the chamber system enabling one to explore SOA formation from the mixture.

For this study, the SOA and ozone forming potential for one FFV-GDI's was analyzed. The vehicle were operated on four different fuels with varying ethanol content (E10, E10 high aromatic, E30, and E78). The vehicles were tested on a cold and hot start, LA-92 driving cycle, both in triplicate. The exhaust was measured to certification standards, and subsequently collected in CE-CERT's 30m^3 Mobile Atmospheric Chamber (MACh) for the entirety of the driving cycle. The emissions were then photochemically aged and real-time particle and gaseous phase measurements were analyzed. Particle instruments include an SMPS, HR-ToF-AMS, VTDMA, and APM. One test in each subset analyzed the secondary aerosol formation of the vehicle exhaust alone. The other two tests, included 1 ppmV of the ROG surrogate in addition to the vehicle exhaust. Results explore secondary aerosol differences due to varying ethanol content, as well as variations due to driving conditions in a simulated anthropogenic environment.

10CB.4

Effects of Adding Gaseous Fuels on the Pollutant Emissions from a Diesel Engine. LIN-CHI WANG, Wen-Jhy Lee, Hsi-Hsien Yang, Jau-Huai Lu, *Cheng Shiu University*

This study used four different gaseous fuels, including H2, imported nature gas (CH4), Taiwan domestic natural gas (90%CH4, 10%CO2) and biogas (70%CH4, 30%CO2), as control measures on fine particulates and other pollutants emitted from heavy diesel engines. Furthermore, diesel particulate filter (DPF) was also deployed to further reduce fine particulate emissions. The percentages of gaseous fuel to total fuel (gaseous fuel + diesel fuel) were 10% and 20%, respectively. The experiments were conducted using a 6-cylinder, heavy-duty diesel engine in a direct-injection mode (Hino W06E), coupled with a dynamometer (Schenck W230) which was used to control the engine torque and speed. The engine had a 6-liter capacity and was water-cooled and naturally aspirated. The diesel engine tests were carried out with three selected modes out of the 13 European Steady Cycles (ESC) modes: mode 1 (idle, 750 rpm, 0 % load), mode 6 (1650 rpm, 270 Nm) and mode 3 (1950 rpm, 96.2 Nm). The influence of these control measures on the physical and chemical properties of particulates from heavy diesel engines were discussed. The results showed that after adding gaseous fuels, the thermal efficiency only declined slightly compared to using diesel as fuel, but NOx was decreased 5-25%, and the reduction of opacity was even higher than 50%. In general, adding gaseous fuels can also reduce emissions of PM2.5, TPM, and PAHs at 75% load which engine efficiency is greater. Except for CH4 gaseous fuels, adding other gaseous fuel with diesel can reduce PAH emissions, especially for H2, which reduce 88% of PAH mass emissions and 50% of PAH BaPeq emissions. Therefore, adding gaseous fuels can be a candidate technology that can both reduce PM (including PM2.5) and NOx at the same time, which is hard to overcome. Although adding gaseous fuels will increase the emission factors of particulate number from heavy diesel engines, DPF can be deployed to remove 99% of non-volatile particulate matter. The optimization of engine operation and combustion condition for gaseous fuels needs to be further studied to ensure pollutants removal and further increase their removal rates.

10CB.5

Characteristics of Particulate Matter and Particle-bound Metal Emissions from a Diesel Engine Generator Fueled with Waste Cooking Oil-based Biodiesel Blended with Butanol and Acetone. Jen-Hsiung Tsai, Jia-Twu Lee, Ciao-Jhen Guo, Kuo-Lin Huang, Sheng-Lun Lin, SHUI-JEN CHEN, *National Pingtung University of Science and Technology*

This study investigates the emission characteristics of particulate matter and particle-bound metals from a diesel engine generator fueled with traditional fossil diesel (D100) with the additions of acetone (A), water-containing acetone (A'), isopropyl alcohol (I), butanol (B), water-containing butanol (B'), or waste cooking oil-based biodiesel (W). The fuel blends were D50W20B30 (abbrev. “B30”), D50W20B'30 (abbrev. “B'30”), D76W20A3I1 (abbrev. “A3”), D76W20A'3I1 (abbrev. “A'3”), D46W20B30A3I1 (abbrev. “B30A3”), and D46W20B'30A'3I1 (abbrev. “B'30A'3”) tested at 1.5 and 3.0 kW loads of the diesel engine generator. Results show that using B30, A3, and B30A3 reduced the PM mass concentration in the exhaust in comparison with using only W20 at both engine loads. Additionally, the PM emission concentrations were lower using B'30, A'3, and B'30A'3 than using B30, A3, and B30A3, respectively; in other words, the PM emission concentrations were further reduced when the acetone was replaced with water-containing acetone in the blends. However, the presence of B30 and B30A3 had more contribution on reducing the PM emissions than that of A3, regardless of the water content in fuel blends. On the other hand, compared with using W20, the metal contents in PM emissions decreased by using B30, B'30, A3, A'3, B30A3, and B'30A'3 at both engine loads. The major metal components in PM were Na, Mg, Al, K, Ca, Fe, and Zn, contributing about 97% of overall 21 metals (in mass). The rest of analyzed metals were dominated by Mn, Ni, Cu, Mo, and Ba. Accordingly, the addition of waste cooking oil-based biodiesel and water-containing acetone/butanol may be considered as one of diesel alternatives for diesel engine generators to reduce PM and PM-bound metal emissions. It is also suggested that waste water-containing acetone/butanol can be used for the recycling purpose in this process.

10CB.7

Combustion Conditions Leading to Primary Brown Carbon Emissions in Diesel Exhaust and Biomass Combustion.

Vilhelm B. Malmborg, Axel C. Eriksson, Sandra Török, Christina Andersen, Louise Gren, Christoffer Boman, Robert Lindgren, Kirsten Kling, Sam Shamun, Martin Tunér, Yilong Zhang, Shawn Kook, Per-Erik Bengtsson, JOAKIM PAGELS, *Lund University, Sweden*

The occurrence of light absorbing carbon (LAC) with enhanced absorption in the UV region (Absorption Angstrom Exponent, AAE >1) is well documented from measurements early in the soot formation process in lab-flames and diesel engines (Malmborg et al. 2017). In the atmospheric community, additional UV absorption is most often discussed in relation to biomass combustion emissions, and is then often referred to as Brown Carbon (BrC). Neither, the combustion conditions resulting in the BrC emission, nor the chemical components responsible for the absorption are well known for real world sources.

In this study we investigated BrC emissions from; 1) a mini-CAST flame soot generator using nitrogen dilution to vary flame height and temperatures, 2) a modern heavy duty diesel engine, operated on diesel and biodiesel fuels, where flame temperatures are varied using Exhaust Gas Recirculation (EGR; a common NOx reduction technique), 3) a Nordic wood stove used for domestic heating, and 4) a natural draft gasifier cookstove using pelletized woody biomass.

The optical properties of the aerosol was characterized with either an Aethalometer (model AE33 Magee Sci.) or a custom made 4-λ diode laser in-situ extinction device. The particle chemical composition was investigated using a Soot Particle Aerosol Mass Spectrometer (SP-AMS). PM was collected on quartz filters for thermal-optical analysis of Elemental and Organic Carbon (EC/OC; EUSAAR 2) and on TEM grids for High-Resolution Transmission Electron Microscopy (HR-TEM) analysis. In select cases a thermal denuder (300 °C) or a high temperature furnace (up to 900 °C) was used to investigate volatile and non-volatile fractions, and the effects of thermal processing on particle composition and optical properties.

The mass absorption cross section values of emissions from the flame soot generator decreased with increasing nitrogen dilution, in accordance with the literature. At the same time the AAE increased from just above 1 to 3.5 and HR-TEM analysis showed that the mean carbon lattice fringe-length decreased. Hence, reducing the flame temperature using N_2 produces less mature, less graphitized, soot. Thermal processing removed semi-volatile OA such as PAHs. However, the AAE was still far above 1.0. The cases with elevated AAE were associated with significant fractions of the aerosol in the OC3-4 channels and “pyrolytic carbon” in the thermal-optical analysis, as well as large carbon clusters in the mid-carbon and fullerene carbon range detected by the SP-AMS.

Similar trends were obtained using increasing levels of EGR in the heavy duty diesel engine. AAE increased from ~1 to 2.5 with increasing EGR and was only partially reduced upon removal of PAHs with the TD at 300 °C. Again elevated fractions of OC 3-4 and pyrolytic carbon were found in the thermal optical analysis for LAC with high AAE.

Emissions from the conventional well insulated wood heating stove showed in general AAE.

A clear trend between primary BrC emissions and combustion conditions is emerging. It appears that BrC emission cannot be assigned to neither the organic fraction, nor the refractory soot core. Instead, BrC is more likely related to the slow rates at which particle properties matures in flames with reduced temperatures.

Finally, it is interesting to note that all of the cases resulting in elevated BrC emissions also resulted in elevated PAH emissions, which suggests these emissions are of health relevance.

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10CB.9

In-Situ Estimation of Non-Regulated Pollutant Emission Factors in Urban Area With Fleet Composition Characterization. SIMON MARTINET, Yao Liu, Liliane Jean-Soro, Mathieu Goriaux, *IFSTTAR*

In urban areas, road traffic is one of the main causes of air pollution. Besides regulated pollutants, the road transport induces also particles, black carbon (BC) and several VOCs and SVOCs (Volatile and Semi-volatile Organic Compounds) emissions which lead to serious negative impacts on human health and air quality inside the cities. This study aims to estimate the emission factors of these different unregulated pollutants in an urban area with real fleet composition and traffic conditions (speed, traffic congestion, and number of vehicles) during 11 days (background and urban dense traffic areas). The particle number concentration and black carbon were measured with FMPS (fast mobility particle sizer), SMPS (scanning mobility particle sizer), and Aethalometer 33-7. The VOC and SVOC were collected using cartridges and quartz filters and analyzed by GC-MS. The urban site is two way street with two directions and limited to 30 km/h with traffic lights. The fleet composition and the traffic conditions were characterized by two cameras and two pneumatic tubes allowing counting the vehicle number, average speed and vehicle type (light-duty vehicles, light-commercial vehicles, heavy-duty vehicles, buses, motorcycles,…) and their characteristics (brand, model, fuel, engine, age, EURO emission standard,…). The road fleet composition characterized during this campaign is representative of French fleet with 90 % of light-duty vehicles, 8 % of light-commercial vehicles, 1 % of heavy-duty vehicles and buses and 0.5 % of motorcycles. For the light-duty vehicles, the repartition according to the fuel is about 32 % of gasoline and 62 % of diesel and the repartition according to the EURO emission standards is about 14 % of EURO 6 vehicles, 30 % of EURO 5, 29 % of EURO 4, 17 % of EURO 3, 7 % of EURO 2 and 2 % of EURO 1. The emission factors vary from 6 to 1800 µg/veh/km for the formaldehyde, from 8 to 8000 µg/veh/km for the toluene, from 1.2×10^{13} to 9.5×10^{14} #/veh/km for the particle number and from 1.7×10^{6} to 2×10^{8} ng/veh/km for the black carbon during 7 days. The evolution of the particle mean diameter were also observed according to the traffic, the wind speed and the traffic mean speed that might be explained by atmospheric physical phenomena (dispersion, coagulation, resuspension…).

10CB.10

Secondary Organic Aerosol Formation Potential of Next-Generation Biofuels. BRANDON KING, Platt Ben, Liam Lewane, Pothier Matson, Delphine Farmer, McCormick Robert, Thornton Matthew, Ratcliff Matthew, Shantanu Jathar, *Colorado State University*

A major anthropogenic source of atmospheric particulate matter (PM) is the transportation sector, specifically motor vehicles. There is a substantial potential to significantly reduce ambient PM levels through the development of better fuels. The Department of Energy's Co-Optima initiative is aimed at developing more sustainable, scalable, and tailpipe-emission friendly fuels. This initiative would reduce direct tailpipe emissions of carbonaceous aerosol (i.e., black carbon and primary organic aerosol) but no consideration is given to the secondary organic aerosol (SOA) formed through the atmospheric oxidation of gas-phase hydrocarbon emissions. Hence, there is a need to quantify the SOA formed from these prospective fuels.

In this work, we performed experiments in a 10 m^3 Teflon environmental chamber to measure the formation and composition of SOA from photooxidation of unburned Co-Optima fuels. We tested four of the eight biofuels identified by the Co-Optima initiative as drop-in substitutes for gasoline. The four biofuels were: Vertifuel (complex mixture of hydrocarbons with 70% aromatics), furan mixture (60:40 weight ratio of dimethylfuran and 2-methylfuran), cyclopentanone, and diisobutylene. The photooxidation experiments were initiated using the hydroxyl radical, which was formed through the photolysis of nitrous acid (HONO) and performed under atmospherically-relevant concentrations of NO_x. The SOA volume concentration was tracked using a scanning mobility particle sizer and the SOA composition was captured using an aerosol mass spectrometer. Preliminary results suggest that all of the biofuels tested had much higher SOA mass yields compared to unburned gasoline. This implied that blending these biofuels with gasoline might lead to increases in ambient SOA in urban areas where motor vehicles account for a significant fraction of the fine particle pollution.

Ongoing work is focused on performing additional experiments with these biofuels to allow parameterizations to be developed for air quality models and using those parameterizations in air quality models to examine the tradeoffs between lower primary emissions and higher secondary production on ambient SOA mass concentrations.

10CB.12

Large Eddy Simulations of Staged Pressurized Oxy-Combustion. FATMA KARAISMAIL, Akshay Gopan, Richard Axelbaum, Ismail Celik, Benjamin M. Kumfer, *Washington University in St. Louis*

Oxy-fuel combustion is one of the popular methods for reducing carbon dioxide emissions from fossil fuel combustion systems. However, a large amount of flue gas recycle is required in oxy-fuel combustion to control the heat flux by lowering the flame temperature, but this poses a significant efficiency burden on the process [1]. In non-premixed oxy-gas combustion systems, the high radiative heat flux results from the large soot volume fraction. One of the ways to control the radiative heat flux is to reduce the soot volume fraction, without compromising on the flame temperature. To do so, the inert can be strategically distributed between oxidizer and fuel to change the stoichiometric mixture fraction, Zst, of the flame, which has been shown to reduce soot and radiative heat flux [2].

In this study, Large Eddy Simulations (LES) will be used to further characterize this suppression of soot inception. The experimental reactor at Washington University in St. Louis is modeled for both methane and propane combustion, and mixture fraction maps are generated to provide the flame structure, which has a strong influence on soot inception within the reactor. The mixture fraction maps are obtained by extracting the corresponding data from arbitrary lines across the turbulent flame for different Zst values at the inlet. The important parameters affecting soot inception, such as the C/O ratio and the temperature limits for soot formation, are calculated by means of a simple model [3]. Parametric studies have been performed and variances over space and time are calculated. The LES results are also compared with Reynolds Averaged Navier-Stokes (RANS) models using the same approach to determine the soot inception regions.

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10CB.13

Self-explosion of Lower Alkanes and Alcohols Fine Droplet at the End of Evaporation. Enomoto Hiroshi, Teraoka Yoshikazu, Hieda Noboru, Ota Yoshihide, UESAWA TOMOKI, *Kanazawa University*

In a usage of the liquid fuel with spray combustion method, a higher fuel pressure is used to produces finer droplets. A finer droplet means a higher droplet number density in the fuel. A developed measurement method with that uses X-ray showed that the Sauter mean diameter of the spray was almost 20 µm. In studies of order to consider the droplet evaporation or combustion, the suspended droplet method is the major method used because the environment could can be easily defined easily. However, it is not easy to investigate droplets of diameter 20 µm because the suspension wire/rod diameters should be larger than 5 µm. The authors developed a single-droplet producer and used the free-droplet method to observe the end of evaporation of 20 µm diameter droplets.

Evaporation of droplets of diameter 20 µm in a high-temperature reducing atmosphere was observed directly with a black/white high-speed camera. A high-speed camera (Photron SA-Z, black/white, 100k fps, 10 µs temporal resolution) with a telecentric lens (VS-Technology, VS-TM10-55CO, 55 mm working distance, 10× magnification) and a rear converter (VS-Technology, SV-2.0X, 2× magnification) was used. The spatial resolution and viewing field area were 1.1 µm/pix and 0.211 mm × 0.275 mm, respectively. A continuous light-emitting diode (SUMITA LS-L109) was used as a backlight. The optical equipment was adjusted so that one droplet locus has more than 50 points (frames). The temporal resolution was 10 µs. A high-temperature reducing atmosphere was produced by a butane diffusion flame of diameter 2.5 mm The butane flow rate was adjusted with a mass flow controller (KOFLOC 8500MC, 0.2 cc/min resolution) and set at 7.0 cc/min at room temperature. The average flow velocity in the outer tube was 0.15 m/s. If Poiseuille flow is assumed, the center flow velocity was 0.30 m/s. The droplet velocities in the observation area were 1.5 m/s near the edge of the outer tube and almost 0.3 m/s near the explosion phenomena. The initial velocity of the droplet varied because a spray gives several droplet velocities. The temperature distribution in the flame was measured with a K-type thermocouple wire of diameter 14 µm. The temperature near the injection tube edge was 315 K, which is lower than the boiling point of gasoline. The maximum temperature of the observed area was 1300 K. Six linear-chain alkanes (99.0% n-heptane, 98.0% n-octane, 98.0% n-decane, 98.0% n-dodecane, 97.0% n-tetradecane, and 97.0% n-hexadecane), four alcohols (99.5% ethanol, 99.7% propanol, 99.0% butanol and 99.0% pentanol) and three commercial fossil fuels (Gasoline No. 2, kerosene, and Diesel oil No. 1) were used.

Except in a few cases, an explosion (self-explosion) was observed. The diameters at the explosion (self-explosion diameter) were 5–10 µm. Larger carbon number alkane gave smaller self-explosion diameters. The initial evaporation rate of faster initial velocity was larger than that of slower initial velocity in any cases. Though the initial evaporation rates of the commercial fuels were almost same at the same initial velocity, these of the alkanes and the alcohols were different with the carbon number. The self-explosion diameters and the initial evaporation rates of the commercial fossil fuels were almost the same for the same initial velocity.

10CB.14

Deconvolution of Nanoparticle Size Distributions Measured in Combustion Processes. HARTMUT MÄTZING, Werner Baumann, Andrei Bologa, Alexandra Loukou, Nadine Teuscher, Petros Vlavakis, Hans-Joachim Gehrmann, Hanns Rudolf Paur, Dimosthenis Trimis, Dieter Stapf, *KIT, Karlsruhe, Germany*

Nanoparticles are frequent by-products in laboratory and industrial scale combustion processes. They may originate from soot formation, from nucleation/condensation of organic material and of evaporated ash, from break-up of agglomerates or just from incompletely burnt material (dust). Depending on conditions, the particle size distributions may exhibit several peaks, e.g. a nucleation and several accumulation modes. Often, these modes overlap and may be difficult to detect by visual inspection. Therefore, numerical tools are required for peak deconvolution. Recently, differential evolution (DE) has been recommended as suitable tool to deconvolute particle size distributions in the µm size range (Alderliesten, 2016). Here, the application of DE to nanoparticle size distributions is demonstrated.

The nonlinear least squares regression code (NLINLS) provided by Mishra (2007) was upgraded from F77 to Fortran 95/2003 and used to generate Fit4LogNorms, an interactive code for fitting up to nine log normal particle size distributions (PSD) to a given dataset. Inputs are the particle size dp [nm or µm], the number density, dN/dlog dp [cm^{-3} or m^{-3}], and some control parameters. The code approximates the user specified number of peaks to the given size distribution and reports the mean particle size, the total particle number density and the distribution width for each peak together with the fit quality. Occasional peak identities are checked and detected according to user specified criteria like minimum difference of mean particle size or size distribution width. The code was tested against literature results (Alderliesten, 2016) and other test cases.

Fit4LogNorms was applied to measurements of selected laboratory and bench scale experiments:

(a) metal oxide particles/agglomerates in flat and conical premixed C_2H_4 and C_3H_8/air flames (Teuscher et al., 2016)
(b) soot formation in flat, premixed, superadiabatic CH_4/O_2 flames (Sentko et al., 2016)
(c) fly ash particles from a 100 kW wood chips boiler (Bologa et al., 2013)
(d) fly ash particles at a bench scale, 2.5 MW wood dust burner (Baumann et al., 2017).

All inspected size distributions were found to be multimodal, containing up to 5 modes. Note in particular that valid extrapolations are applicable to size distributions which are incomplete because of experimental limitations or for other reasons.

These examples show that in lab as well as bench scale applications aerosol dynamics is very complex. The multiple mode size distributions may be due to simultaneous nucleation, condensation, coagulation and heterogeneous reactions. In addition, the particle sampling process itself may affect the size distribution, especially under highly reactive conditions. Peak deconvolution can deliver key information for a full understanding of the aerosol formation and behavior.

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10CB.15

Effect of Soot and Radiation Models in Prediction of Pollutant Formation from Practical Combustion Scenarios.

KHALED MOSHARRAF MUKUT, Somesh Roy, Sebastian Ferreyro Fernandez, Daniel Haworth, Michael Modest,
Marquette University

Soot or black carbon is one of the major contributors to global climate change, yet there remains a large uncertainty in our understanding of formation and evolution of soot. Anthropogenic combustion is a major source of soot. While combustion research had advanced dramatically over the last couple of decades, formation and growth of soot from real-world combustion scenarios are still poorly understood because of computational complexity and multiphysics interactions involved.

Detailed modeling of combustion requires accurate modeling of flow, chemistry, soot and pollutant formation processes, and thermal radiation. In this work, we focus on soot and radiation modeling in complex combustion configurations. There have been numerous studies on detailed soot modeling in laboratory-scale flames with simple configurations. However, these studies are often restricted to low-sooting conditions. Modeling of thermal radiation is, on the other hand, often simplified either because of numerical complexity or its relatively small importance in small-scale laboratory flames. However, recent studies show that effect of radiation cannot be overlooked in moderate-to-highly sooting flames, high-pressure combustion, and large-scale combustion configurations. To explore the effect of soot and radiation modeling and their interaction we performed detailed simulations of Diesel engine-relevant configurations based on high-pressure Diesel spray experiments reported at Engine Combustion Network (ECN). A semi-empirical and a moment-based detailed soot model with detailed chemical kinetics are used in the coupled simulations of the target cases. A high-fidelity line-by-line photon Monte Carlo and simple gray models have been used for radiation modeling. The primary objective of this work is to explore the effect of model empiricism and interconnection of soot and radiation modeling in practical combustion configurations. Coupled simulations with both detailed and simple soot and radiation models indicate a strong interdependence between soot and radiation models. Significant differences in both size and volume fraction of soot are noted due to the fidelity of the radiation modeling. Apart from the direct connection between predicted soot population and thermal heat loss, the effect of model empiricism on other relevant indicators such as the production of large PAHs and NOx are also quantified.

10CB.16

Structure and Size of Carbon nano-Particles Generated in Laminar Premixed Flames. MARIO COMMODO, Gianluigi De Falco, Patrizia Minutolo, Andrea D'Anna, *IRC-CNR, Napoli, Italy*

The physicochemical properties of flame-generated carbon nanoparticles are investigated in a set of ethylene/air premixed flames with the objective of highlighting the peculiar characteristics of the particles produced across the transition from a mono-modal to a bi-modal particle size distribution.

Particle size distributions are measured by differential mobility analysis, while particle structure and composition are retrieved by Raman spectroscopy, UV–vis light absorption, X–ray and ultraviolet photoemission spectroscopy. Particle morphology is instead obtained by atomic force microscopy measurements.

Experimental results show that by increasing the flame residence time and equivalence ratio, particle size moves from a mono-modal, i.e., only nucleation-mode particles are formed, to bi-modal distribution when also an accumulation mode of particles is present. The change of the average particle size and the shape of the size distribution is associated to a strong change of the particle physicochemical properties. The combination of different analytical methods demonstrates that in richer flames the particles become more graphitic as the three-dimensional clustering of the aromatic planes proceed. Nevertheless, Raman spectroscopy shows evidence of a larger structural disorder in the accumulation mode particles as compared to the nucleation particles. This is most likely due to lattice distortion caused by the formation of five membered rings on the growing edges of the aromatic layers.

10CB.17

Effect of Acetone-Butanol-Ethanol (ABE) Addition to Diesel on the Soot Formation and Soot Reactivity. JIANFEI LUO, Yongming Zhang, Qixing Zhang, *University of Science and Technology of China*

Soot particles from vehicles, especially diesel vehicles is a significant contributor to atmospheric PM2.5, it is very necessary to increase the adoption of oxygenated fuels as alternative fuels to reduce pollutant emissions.Acetone-Butanol-Ethanol (ABE), the intermediate product in bio-butanol production process using biological fermentation purification technology, has been proposed to blend diesel directly for saving the high energy requirement of separating purity butanol. Literature has shown that ABE has a similar combustion characteristics in engine compared to petroleum diesel. This work aims at understanding the soot formation in ABE-diesel blends diffusion flame, and the oxidation reactivity of ABE-diesel blends derived soot.

The Threshold Sooting Index (TSI) calculated from fuel consumption rate and smoke point were used to evaluate the sooting tendency of ABE-diesel blends. And the results indicated that the normalized TSI showed a cutting down exponent trend with increasing concentration of ABE in diesel, embodying the emission reduction capacity of ABE. To reveal the inhibitory nature of soot formation in ABE blends flame. Toluene and heptane were selected as model alternative fuels for diesel to establish the ABE blends chemical reaction mechanism. The laminar premixed flame structure of ABE-toluene-heptane blends were calculated through CHEMKIN Pro. It was found that the concentration of toluene were diluted in premixed zone and were consumed ahead of high temperature zone, thus the concentration of soot precursors such as polycyclic aromatic hydrocarbons (PAHs) produced in the presence of toluene were decreased. The amplification effect of smaller PAHs polymerization reaction further reduced the larger PAHs generation rate. In addition, the increased HO2 and OH concentration by ABE accelerated the oxidation consumption of PAHs.

To characterize the oxidation reactivity and physicochemical properties of ABE-diesel blends derived soot. Several diagnostic experimental technologies such as Thermogravimetric analysis (TGA), Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and high resolution transmission electron microscopy (HRTEM) have been used. It was observed that the average activation energies of ABE-diesel blends derived soot were lower than diesel derived soot. And the variation in the sizes of primary particles, fringe length, fringe tortuosity, the amount of functional groups, atomic O/C ratio, and H/C ratio support the higher oxidative reactivity of ABE-diesel blends derived soot.

10CB.18

Investigating the Dependence of Light-absorption Properties of Combustion Carbonaceous Aerosols on Combustion Conditions. ZEZHEN CHENG, Khairallah Atwi, Daniel Tarquinio, Rawad Saleh, *University of Georgia*

The light-absorbing components of organic aerosols emitted by incomplete combustion, collectively referred to as brown carbon (BrC), exhibit highly variable light-absorption properties, usually quantified in term of the wavelength-dependent mass-absorption cross-section (MAC). The wavelength dependence of MAC is quantified in terms of the Absorption Ångström Exponent (AAE). There are two major reasons for the variability in BrC's MAC and AAE: 1) BrC is a collection of poorly characterized compounds, and thus the reported MAC and AAE values depend on which of these compounds are featured in a particular measurement, which in turn depends on the combustion conditions associated with the measurement; and 2) BrC is often co-emitted with black carbon (BC), complicating the retrieval of its MAC and AAE due to the overlap of light absorption by the two components, thus leading to discrepancies between different approaches employed to achieve this retrieval.

To address these challenges, we designed controlled combustion experiments that enabled us to isolate BrC components with varying light-absorption properties, as well mixtures of BrC and BC. Combustion was performed under steady-flow conditions in a temperature-controlled quartz chamber. Different combustion conditions were achieved by varying the chamber temperature and the relative flowrates of air and fuel. We also used an extra stream of nitrogen as a passive diluent to fine-tune the combustion conditions. Adding a passive diluent has a similar effect on the products as making the combustion more fuel rich. We calculated the wavelength-dependent MAC of the emissions from real-time absorption coefficient measurements using a 3-wavelength (780, 532, and 420 nm) photoacoustic spectrophotometer and an Aethalometer and integrated size distribution measurements using a scanning mobility particle sizer.

We used benzene and toluene as model fuels. Starting with relatively low-temperature and fuel-rich combustion experiments and progressively increasing the temperature and/or the air/fuel ratio, we produced carbonaceous aerosol samples with progressive change from weakly absorptive BrC (MAC at 532 nm ~ 0.22 m2/g and AAE ~ 8) to highly absorptive BrC (MAC at 532 nm ~ 2.0 m2/g and AAE ~ 3) to mixtures of BC and highly absorptive BrC (MAC at 532 nm ~ 3.0 m2/g and AAE ~ 1.5). These results cover the wide range of values reported in the literature and indicate that the carbonaceous aerosol light-absorption properties depend strongly on combustion conditions.

We also attempted to obtain correlations between the light-absorption properties and two indicators of combustion conditions: the modified combustion efficiency (MCE = $\Delta CO_2 / (\Delta CO_2 + \Delta CO)$) and the organic to total carbon ratio (OC/TC). CO and CO_2 concentration were measured using FTIR and OC/TC was measured offline using an OCEC Analyzer. We found stronger correlations between MAC at 532 and AAE with OC/TC than with MCE, indicating that OC/TC is a better predictor of light-absorption properties than MCE.

10CB.19

Characterization of a New MiniCAST Generator (Model 5201 Type BC) Offering Both Diffusion and Premixed Flame Option. MICHAELA N. ESS, Konstantina Vasilatou, *METAS*

Black carbon (BC), light-absorbing carbonaceous substances in atmospheric aerosol [1], is known to have a huge impact on climate as well as on the human health. It is generated by combustion of natural as well as anthropogenic origin. With the potential of causing diseases, direct influence on the earth's radiation budget and also indirect effects e.g. as cloud condensation nuclei, BC is one of the atmospheric components strongly monitored.

Optical absorption methods, filter based as well as filter free ones, are normally used for the monitoring of BC. Since for common filter-based methods the measurement is affected by the filter type and particle properties, the application of a general calibration factor is impossible. To apply a standardized calibration for specific particle types, standard aerosol sources generating particles with well-defined physical parameters, which can be used to quantify aerosol absorption with traceability to primary standards, are needed. The development and characterization of such sources in one of the goals of the EMPIR 16ENV02 Black Carbon project.

In this context, we are investigating the optical, physical and chemical properties of the carbonaceous aerosols produced by the new miniCAST soot generator Model 5201 Type BC (Jing Ltd.). In contrast to former CAST models, which rely entirely on diffusion flames of a fuel (often diluted with nitrogen) and air, the new model offers the possibility of:

i) adding air instead of nitrogen to the fuel (in this case propane gas) to achieve different levels of premixing;
ii) adding oxygen to the oxidation air;
iii) adding oxygen to the quench gas.

Although a completely premixed flame is not possible because the (premixed) propane is still surrounded by an oxidation air cone causing also diffusion flame conditions, the versatility of the new miniCAST model offers further possibilities to tune the properties of the generated BC particles.

These are analyzed with respect to their size, number and mass concentration using an SMPS and a TEOM, while an Aethalometer is used to determine the BC mass concentration and the Ångstrom absorption exponent α. Additionally, the microstructure and the chemical composition of the particles is characterized with micro-Raman Spectroscopy and OC/EC analysis, respectively.

By operating the new miniCAST with a normal diffusion flame, particles with geometric mean diameter (GMD) up to 180 nm can be achieved with improved stability and reproducibility compared to older models. While at overall fuel rich conditions the EC content decreases fast with decreasing particle size, at fuel lean conditions also smaller particles (GMD ≥ 65 nm) with high EC content (≥ 85 %) and low α (≤ 1.4) can be generated even without volatile particle remover.

Using the premixing option, smaller particles were generated at the same overall fuel-to-air ratio compared to the pure diffusion flame. Thereby it seems to be possible to also generate particles with GMD ≥ 30nm and increased BC fraction compared to older CAST models.

In this work, a detailed characterization of the aerosol properties at different operation points of the CAST generator will be presented.

This work is part of the 16ENV02 Black Carbon project funded by the European Union through the European Metrology Programme for Innovation and Research (EMPIR).

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10CB.20

Prevention of Back Corona Discharge Luminescence in an Electrostatic Precipitator Using Asymmetrical Rectangular AC Voltage. TOMOYA MITSUI, Koji Yasumoto, Akinori Zukeran, Takashi Nakano, Koyu Tsubouchi, Takashi Ogawa, *Kanagawa Institute of Technology*

An electrostatic precipitator (ESP) has been extensively used for removal particulate matter. However, when particles which has high resistivity deposit on dust-collection electrodes, back corona discharge is generated, and the dust-collection performance decreases. Therefore, the aim of this study is to prevent back corona discharge using asymmetrical rectangular AC voltage.

The experimental ESP consisted of a high-voltage application wire electrode (tungsten,Φ0.26) and a grounded plate electrode (90×150 mm) with the gap of 15 mm[1)]. Calcium carbonate dust (thickness: 0.5 mm) was located on the surface of the grounded plate electrode. Symmetric or asymmetric rectangular AC voltages (voltages: ±9 kV) were applied to the wire electrode. The voltage waveform and the current waveform were measured, and a photograph of discharge luminescence on the surface of the dust layer was taken by a digital camera.

As a result, when the symmetric rectangular AC voltage was applied, the current for the time between 0 and 12.5 ms was approximately 0.01 mA due to corona discharge during the positive polarity. However, the current increased with elapsing the time after 12.5 ms due to back corona discharge. During the negative polarity, the tendency was similar with the positive polarity.

Therefore, an asymmetric rectangular AC voltage with the positive polarity application time of 7 ms and the negative polarity application time of 2 ms (the total period: 9 ms) was applied to the wire electrode to prevent the increasing the discharge current. The discharge current did not increase in both the positive and the negative polarities in the results.

The back corona discharge luminescence on the surface of the dust layer were taken by a digital camera, when the symmetric and the asymmetrical rectangular AC voltage were applied. The back corona discharge luminescence was observed on the surface of the dust layer in the symmetrical rectangular AC voltage. On the other hand, the luminescence was not observed in the asymmetrical rectangular AC voltage.

These results indicated that the back corona discharge was prevented due to applying the asymmetric rectangular AC voltage, whereby the discharge current did not increased.

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10CB.21

Numerical Analysis of Electric Field Distribution in Wire-to-plate Type Electrostatic Precipitator. KOHEI ITO, Akinori Zukeran, Yoshihiro Kawada, Tomohiro Taoka, Kenji Shibata, *Kanagawa Institute of Technology*

Electrostatic precipitator (ESP) has been used for exhaust gas purification in order to suppress air pollution. Numerical analysis is effective for development of ESP. In this study, the electric field distribution under corona discharge in a wire-to-plate type ESP was analyzed using general purpose finite element method analysis software COMSOL Multiphysics® Ver.4.3b, and the result was fitted to the experimental result.

A two-dimensional model of wire-to-plate type ESP was calculated. The gap between the wire electrode (Tungsten, ϕ=0.26 mm) and the grounded plate electrode (Stainless, L=40 mm) was 15 mm. The space was the air, a potential of -10 kV was applied to the surface of the wire electrode, and the surface of the grounded plate electrode was 0 V. The ion density of 4.53×10^{15} m^{-3} was given to the surface of the wire electrode, and the other boundaries were 0 m^{-3}. The ion density on the surface of the wire electrode was adjusted, whereby the calculated peak value of the current density distribution on the surface of the grounded electrode was equal to the experimental value. The number of the mesh division was approximately 400 thousand. The fundamental equations are Poisson equation (1) and negative ion continuous equations (2):

$$-\nabla\cdot\varepsilon_r\varepsilon_0\nabla V=\rho \quad (1)$$
$$\partial N_n/\partial t+\nabla\cdot(-D_n\nabla N_n-\mu_n E N_n)=0 \quad (2)$$

where ε_r is the relative permittivity, ε_0 is the dielectric constant of vacuum, V is the potential, ρ is the space charge density, D_n is the diffusion constant of negative ion, μ_n is the mobility of negative ion and E is electric field. The space charge density ρ is obtained from the following equation.

$$\rho=-eN_n \quad (3)$$

where e is elementary charge and N_n is the negative ion density.

The electric field intensity near the surface of the wire electrode was the highest of approximately 1×10^7 V/m, and the intensity has minimum value at the location between the wire electrode and the grounded plate electrode. The electric field intensity at the center on the surface of the grounded plate electrode was high due to space charges, and that decreased with increasing the distance from the center. The discharge current was calculated from the electric field intensity near the surface and the ion density, which were calculated by finite element method as following equation:

$$I=\rho\mu_n ER \quad (4)$$

where I is the discharge current, R is the circumference of the wire electrode. The calculated discharge current was 0.901 mA/m, which was almost equal to the experimental value of 0.875 mA/m. This result indicates that the electric field distribution calculated using COMSOL Multiphysics is validity.

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Keywords
Simulation, Corona Discharge, Electric Field, Electrostatic Precipitator.

10CB.22

Investigation of Power Absorption on Combustion of Carbon Black Using Microwave. SOMA TOGUCHI, Akinori Zukeran, Hiroyuki Toyozumi, Takashi Inui, *Kanagawa Institute of Technology*

Particulate substances containing a large amount of carbon black are emitted from ships and diesel generators. Therefore, an electrostatic precipitator (ESP) has been developed to remove them. In order to function at high efficiency, it is necessary to wash the electrode collected dust. In an ESP for a power plant, etc., this cleaning is achieved by mechanical impact rapping or water washing. However, there is a problem such as large-scale apparatus. In this study, the experiments were carried out to burn carbon black using microwave. The power absorption and the combustion rate were investigated.

The system consists of a microwave oscillator, a coaxial waveguide converter, 3 stub tuner, a waveguide and a short plunger. The dimension inside the waveguide was 54.6 mm in height by 109.2 mm in width. A short plunger was installed at the end of the waveguide, and standing wave with a wavelength of 147.9 mm was generated. The distribution of microwave in the waveguide was calculated using CST STUDIO SUITE. The carbon black (APPIE, JIS Z 8901) in porcelain crucible was located in the waveguide. The maximum point of the magnetic field is 74 mm from the short plunger, and that of the electric field is 37 mm and 111 mm. The microwave was irradiated for 5 minutes. The power absorption into carbon black was calculated from the difference between the input power and the reflecting power displayed on the oscillator. The combustion rate was calculated by equation (1).

$$\eta=(1-M/M_0)\times 100\% \quad \cdots(1)$$

where M_0 is the mass of carbon black before irradiation, and M is mass after irradiation.

As a result of relationship between power absorption and location, the power absorption had large values at the distances of 37 mm and 111 mm, where were maximum point of electric field intensity. This result indicate that carbon black absorbed the energy of electric fields more than magnetic field. As a result of relationship between combustion rate and location, the combustion rates were between 11 % and 16 % at any location, especially the rates at the locations of 55.5 mm and 111 mm were greater than the other locations. Therefore, it was found that carbon black can be heated by both electric field and magnetic field, and burned at any location in this experimental condition.

10CB.23

Development of Diesel PM Combustion Reactor using Plasma Assisted Catalysis. HITOMI KAWAKAMI, Takashi Inui, Hideyuki Nishida, Hirotaka Miyasita, Yoshiyasu Ehara, *Fuji Electric Co.*

The particulate matters (PMs) emitted from marine diesel engine exhaust during the combustion process have low resistivity and extremely small in the range of 70-120nm. These particles cause a various human health and environment impacts. After MARPOL 73/78 Annex VI by International Maritime Organization, shipping-induced NOx and SOx, PM emissions are regulated stricter. This research has been developed an after treatment system for removal of diesel PM from the ship exhaust. The PM was combusted by using plasma assisted catalysis. Non-thermal plasma (NTP) reactor had a coaxial double tube structure. The pellets as a catalyst are packed between the inner and outer tubes. A high-frequency voltage was applied to the reactor, NTP was generated. In the NTP reactor, the air is activated by discharge and produces ozone, oxygen radical and nitrogen radical, resulting the diesel particulates are oxidized under low temperature condition. Diesel PMs are perfectly combusted by ozone produced in NTP. When the gas temperature is higher than 250 degrees, NO in the flue gas is oxidized to form NO_2 by ozone and O radical, then carbon particles can be combusted by a reaction with NO_2. Moreover, PMs are also combusted by oxidation catalyst. The catalyst used was NS-1A (Nikki-Universal., LTD.). It is spherical and the diameter is about 4mm. In this experiment, the catalysts surfaces depositing the PM were filled into the reactor. PM is taken from the diesel generator was operated with light oil. In the combustion experiment, plasma was generated in the heater which carried out temperature adjustment. It is thought that PMs combust and generate CO and CO_2. Therefore, CO and CO_2 concentrations before and after the PM combustion were measured and combustion efficiency was determined. From the experimental result, PM combustion efficiency improved by using plasma assisted catalyst. This result shows that the synergistic effect by the plasma and the catalyst can be expected.

10CB.24

Particle Behavior Analysis of Re-entrainment Phenomenon in Electrostatic Precipitator. YOSHIYASU EHARA, Hirotaka Miyasita, Satoshi Kokubu, Hitomi Kawakami, Takashi Inui, Hideyuki Nishida, *Tokyo City University*

The particulate matters (PMs) emitted from diesel engine exhaust during the combustion process have low resistivity and extremely small in the submicron range. An after-treatment system using an electrostatic precipitator (ESP) for removing PM emissions from a diesel engine has been studied. However, the collection of low resistive particles is difficult by the conventional ESPs. The low resistive diesel engine particles are detached from the collection electrode, which causes the particle re-entrainment, resulting in poor collection efficiency. In this study, particle image velocimetry was used especially to analyze the ionic wind and particle behavior in ESP. The ESP model was made of clear acrylic. The high voltage electrode was a stainless needle electrode, and the ground electrode was a plate electrode. It became possible to visualize the re-entrainment phenomenon as a result of the experiment. The discharge current characteristics and the movement angle of re-entrainment particles were investigated.

10CB.25

Identification of Packaging Waste and Catalytical Soot Removal Powder Tracers in Masonry Heaters using Ash and Filter Analyses.

MAREK MAASIKMETS, Hanna Lii Kupri, Alar Konist, Erik Teinemaa, *Estonian Environmental Research Centre*

There is an urgent need to improve understanding the effects of solid waste burning on the air quality, public health and potential impact on climate change (Kawamura et al. 2010). Household waste burning can be an important organic aerosol source. Currently, this source is not included in most emission inventories, and there are only few studies available (Mohr et al. 2009).

Plastic materials cover the biggest fraction of the composition of municipal solid waste. Major compound in smoke from burning plastics include terephthalic acid used predominantly in beverage bottles and similar containers etc. The specific key oraganic tracer for burning of plastics found in atmospheric particle samples also include 1,3,5-triphenylbenzene, which occurs in regions where plastic waste is burned (Simoneit et al. 2005). This suggests that waste composition is largely composite of plastic material, and such waste burning can be traced using the characteristic species detected in the smoke of plastics and refuse burnings (Kumar et al. 2015). Currently, there are only few studies related to tracers for plastic waste burning aerosols.

According to the members of Estonian Chamber of Chimney Sweepers evaluation, in addition to the wood, paper and cardboard waste, people also tend to burn Tetra Pak's, sanitary napkins, diapers, various plastic packages, shoes, textile etc. According to the Fire Safety Act, Estonians need to request certified chimney sweeper services at least once during a period of five years. However, it has emerged that during the five year period some people have started to use uncertified means in a form of burning soot and tar removal catalytic powder and -bricks in order to maintain the oven and chimney. These means do not have a composition list on the package to inform the users, but they consist different kind of metal salts and copper, which is known to favour PCDD/F formation. The environmental impact of such catalytic soot removing means has not been analysed thoroughly and usage is not regulated at the EU level.

Methods and results

In this research we have measured emissions from the modern masonry heater, which occur during catalytic soot removing powder and -brick combustion. 3 types of experiments were conducted in the Estonian Environmental Research Centre's stove laboratory. First experiments included combusting pure conifer and hardwood logwood. Conifer, hardwood logwood and soot removing powder experiments were conducted in two ways: 1. burning conifer, hardwood logwood and including weighted soot removing powder in three stages throughout the combustion process; 2. burning conifer, hardwood logwood and sprinkling the soot removing powder over the wood before the ignition. During the conifer, hardwood logwood and soot removing powder experiments, the powder was placed inside the oven before the ignition.

All particle and gas samples were taken from the hot flue gas. For the particle size distribution and number concentration measurements ELPI+ (10 l/min, (Dekati Ltd) was used. Gas samples (O_2, SO_2, NO, NO_2, CO, CO_2, HCl, HF, VOCs), temperature (°C), H_2O (%) and gas flow (m/s) were measured simultaneously during the whole burning process. For the filter sampling Dekati PM10 impactor was used. Bottom ash samples were collected and stored after every experiment. From sampled filters and bottom ash terephthalic acid was extracted by sonication-assisted solvent extraction and then analyzed with liquid chromatography tandem mass spectrometry (LC-MS/MS). Chromatography was performed on a reversed phase column with methanol and 0.1% formic acid as chromatographic eluents. In addition the chemical composition analysis of bottom ash and filter samples was done using a Rigaku ZSX Primus II WD-XRF spectrometer with 4kW tube and 30micron Beryllium window.

In this research we have found that the combustion of catalytic soot removing means have a significant effect on RWC air emissions and using specific markers it is possible to identify whether waste or soot removal powder in masonry heater was burned.

This work was supported by Estonian Environmental Investment fund.

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10CB.26

Application of Fisher Ratio and Principal Component Analysis for Identification of Unique Features in Complex Combustion-Emission Samples. CHRISTOS STAMATIS, Lindsay Hatch, William Lichtenberg, Georgios Karavalakis, Patrick Roth, Jiacheng Yang, Kelley Barsanti, *University of California, Riverside*

In this work the application of chemometric data analyses is explored for identifying similarities and differences in the chemical composition of combustion emissions that may be linked to the formation of secondary organic aerosol (SOA). Emissions from gasoline combustion have a significant impact on the environment both locally and globally through the production of fine particulate matter (PM). U.S. gasoline blends contain hundreds of compounds, which through incomplete combustion can produce as many products. Many of these products can serve as precursors to SOA, a major mass fraction of fine PM in the atmosphere. Thus, there is motivation for understanding the linkages between fuel composition, combustion emissions, and SOA formation. Advanced instrumental techniques have been critical for increasing the number of compounds identified in complex combustion samples, including those that are most likely to serve as SOA precursors; however, the large data output from such techniques and the complexity of combustion samples, make data processing challenging and time consuming. Chemometric data analysis techniques are increasingly being used to enhance the information that can be obtained through data processing and analysis. As a complement to traditional data analysis, these approaches can lead to improved understanding and model representation of complex processes, including oxidation of gasoline combustion emissions to form SOA.

A MATLAB-based algorithm was developed for preparing and statistically analyzing two-dimensional gas chromatography with time-of-flight mass spectrometry (GC x GC-TOFMS) data. The algorithm performs the following operations: 1. aligns GC x GC-TOFMS chromatograms, 2. calculates Fisher ratios, and 3. performs principal component analysis (PCA) on compounds selected using the Fisher ratios. This algorithm has been applied to gasoline combustion samples collected onto dual-bed absorbent tubes and analyzed using GC x GC-TOFMS. Eight different fuels, with varying aromatic and ethanol content, were tested on a gasoline direct injection vehicle over the LA92 driving cycle; emissions over the entire driving cycle were diluted using a constant volume sampler (CVS) and injected into a mobile chamber where they were oxidized and SOA formation was measured. The Fisher ratio and principle component analyses were performed on samples collected from the CVS and the mobile chamber (prior to oxidation). Details of the algorithm and results of the chemometric analyses will be presented, including implications for better predicting the linkages between fuel composition, combustion emissions, and SOA production.

10DU.1

Early Stage Sub-Micron Particle Formation during Pulverized Coal Combustion in Two-Stage Flat Flame Burner.

DISHANT KHATRI, Adewale Adeosun, Akshay Gopan, Zhiwei Wang, Richard Axelbaum, *Washington University in St. Louis*

In pulverized coal burners, coal particles transition from a short period of locally reducing environment, caused due to the fast release of volatiles from a dense region of coal particles, to an oxidizing environment. This “reducing-to-oxidizing” transition can influence combustion processes such as ignition, particulate formation, and char burnout. Traditionally, fundamental studies on coal combustion have been conducted in systems which neither capture the “reducing-to-oxidizing” transition nor the high a heating rate of practical combustors. In this work, the formation and evolution of sub-micron particles are investigated in a novel two-stage flat flame burner that simulates the “reducing-to-oxidizing” transition and with heating rates on the order of 105 K/s. The particle size distribution (PSD) of the sub-micron particles, and their composition are measured using SMPS and SEM-EDX, respectively. Measurements are carried out under both an oxidizing environment (20% oxygen) and a “reducing-to-oxidizing” environment at two different nominal gas temperatures (1300 K and 1800 K), and three residence times (15, 30 and 60 ms). To differentiate between soot and mineral matter, the SMPS is operated in a tandem fashion, with a high-temperature furnace between the two SMPS measurement locations. The furnace is supplied with a sufficient amount of oxygen to burn off soot in the sampled aerosol stream. The results, including the difference between the oxidizing and reducing-to-oxidizing environments, will be discussed.

10DU.2

Coal Carbonisation for Control of Emissions from Cook Stoves. Darpan Das, Suryendu Dutta, Upendra Bhandarkar, VIRENDRA SETHI, *IIT Bombay*

Volatile matter content of coal has been reported to have a direct influence on the PM2.5 emissions from domestic cook stoves. In the present study two sub-bituminous coals were carbonized at different temperatures to obtain batches of coal samples with different volatile content. These coal batches were then used in a traditional cook stove and PM2.5 emissions were measured. A direct relationship was observed between the volatile matter content of the coal samples and the PM2.5 emissions, suggesting that carbonization of coal could be an immediate strategy to control emissions from coal based domestic cook stoves. However, volatiles-free metallurgical coke was found to be difficult to ignite using the procedure normally used for such stoves. Previous studies also report ignition temperatures to be a function of volatile content. Characterization of the volatiles for different carbonization temperatures was carried out using pyrolysis-GCMS to understand the kind of organics emitted at different carbonization temperatures. The results provide an alternate strategy for control of cook stove emissions, especially in coal mining areas where use of raw coal for domestic cooking is ubiquitous.

10DU.3

Operating Characteristics of Residential Wood Heaters for Emission Measurement. REBECCA TROJANOWSKI, Thomas Butcher, George Wei, Yusuf Celebi, Jake Lindberg, *Brookhaven National Laboratory*

The increased use of wood as a heating fuel in residential buildings has increased concern about the potential environmental health and safety impacts. The increased use is partially due to the historically cheaper cost of wood fuel, but also because the technology offers a renewable alternative to fossil fuel heating. In addition, single room heaters using either pellets or cordwood can help offset significant amounts of home heating oil or propane without the larger investment of replacing a boiler. While wood is seen as carbon neutral fuel and considered to be an important player in the transition to renewable fuel sources, it suffers from higher particulate matter (PM) emissions in comparison to oil or natural gas fired systems.

As of 2015, residential wood combustion (RWC) devices were responsible for more than 45% of PM2.5 (particles with an aerodynamic diameter < 2.5µm) in Europe. Similarly, biomass burning in the United States (US) accounts for more than one-third of primary PM2.5 emissions and the US Environmental Protection Agency (EPA) lists the three largest sources of PM2.5 as utility fuel, RWC and prescribed burning (land management tool to maintain forest health). Specifically in New York State (NYS), residential wood heating contributes 275% more PM2.5 than all industrial, commercial and institutional (ICI) heating emissions combined, 550% more PM2.5 than the electricity generation sector, and 35% more PM2.5 than the transportation sector; overall, contributing more than 90% of the PM2.5 emissions in NYS even though it only provides less than 2% of NYS overall heating needs.

With incentive programs across the world (primarily Europe and North America; specifically in New York State (NYS) - Renewable Heat New York (RHNY) that promote the use of biomass as a renewable fuel source, it becomes very important that we are aware of how wood smoke contributes to ambient air quality. In order to provide information to regulatory agencies, Brookhaven National Laboratory (BNL) has partnered with the New York State Department of Health (NYSDOH) and New York State Department of Environmental Conservation (NYSDEC) to characterize the emissions from a variety of residential wood heating devices. These devices include stoves and boilers; conventional and more innovated modern units that have been operated in a manner which is more reflective of in-field use. Specifically, this work focuses on the operating practices of the heating units and why these practices are so important for emission characterization.

10DU.4

Semi-Volatile Organic Compounds in Fresh and Laboratory-Aged Biomass Burning Aerosols. DEEP SENGUPTA, Vera Samburova, Chiranjivi Bhattarai, Michealene Iaukea-Lum, Adam Watts, Hans Moosmuller, Andrey Khlystov, *Desert Research Institute*

Semi-volatile organic compounds (SVOCs) in fresh and atmospherically-aged biomass-burning aerosols can adversely affect human health and modify radiative forcing of climate. In the present study, we have selected representative fuels (both globally and regionally important) that have characteristics of both flaming and smoldering combustions and burned them under controlled conditions using DRI's combustion chamber facility. Gas and particulate phase emissions from the selected fuels were aged (5-7 days equivalent of atmospheric aging) using an oxidative flow reactor (OFR, Aerodyne PAM). Fresh and OFR-aged biomass-burning aerosols were collected on TIGF filters followed by XAD-4 resin cartridges and extracted with dichloromethane followed by acetone. The extracts were then analyzed for more than 200 compounds (e.g. n-alkanes, polycyclic aromatic hydrocarbons (PAHs), and polar organic compounds) using gas chromatography mass spectrometry technique (GC/MS). Relative abundance of n-alkanes, PAHs, and polar compounds, such as mono- and di-carboxylic acids, and methoxylated phenols, are useful for identifying source profiles of tested fuels. We will present source profiles of combustion emissions generated using individual fuels and discuss how atmospheric aging affects chemical composition of these emissions.

10DU.5

Chemical Composition of Cookstove Emissions: Laboratory Tests and Real-World Use of Traditional and Improved Stoves. ALEXANDRA LAI, Ming Shan, Sierra Clark, Ellison Carter, Kun Ni, Hongjiang Niu, Xudong Yang, Jill Baumgartner, James Schauer, *University of Wisconsin-Madison*

Growing toxicological and epidemiologic evidence indicates that the health effects of exposure to fine particulate matter ($PM_{2.5}$) depend on particles' chemical composition. Inefficient household biomass combustion is a major contributor to personal air pollution exposures for at least three billion people worldwide. However, field studies of household biomass burning that measure $PM_{2.5}$ mass do not typically analyze its chemical composition, which is likely to vary due to factors including fuel type, combustion conditions, stove design, and use of multiple stoves. Consequently, more research on the chemical composition of biomass burning emissions in the field, and how this relates to laboratory measurements, is needed.

Here we investigate the effects of stove and fuel types on composition of $PM_{2.5}$ emissions using both household measurements of real-world stove use and laboratory emissions testing. Field samples were obtained as part of a household energy intervention study in rural Sichuan province, China. Household $PM_{2.5}$ samples were collected on Teflon filters, which were then analyzed either individually (for mass, black carbon (BC), water-soluble organic carbon (WSOC), and water-soluble ions) or in composites (elements by ICP-MS and organic molecular markers, including levoglucosan and polycyclic aromatic hydrocarbons (PAH), by GC-MS). Samples were selected and grouped/composited based on stove use, measured using real-time temperature data loggers. Stove use categories included exclusive and combined uses of traditional, semi-gasifier, and other non-biomass (liquefied petroleum gas, biogas, or electricity). In laboratory emissions tests, samples were collected on both Teflon and quartz filters and the same analyses were conducted as for the field samples, as well as thermal-optical measurement of organic and elemental carbon.

In the laboratory, $PM_{2.5}$ emissions from traditional and semi-gasifier stoves were strikingly different: though both were burning wood, the traditional stoves emitted primarily carbonaceous $PM_{2.5}$, while the semi-gasifier stove emissions were comprised mostly of water-soluble inorganic ions. Preliminary field data reflects similar trends: WSOC and BC account for larger fractions of $PM_{2.5}$ mass when traditional stoves are used. Additionally, summed PAH concentrations comprised a larger fraction of $PM_{2.5}$ mass in households that used traditional stoves than in those that did not, by up to an order of magnitude.

Results from this research will describe how stove design affects emissions independently of fuel type and the extent to which laboratory tests translate to real-world use. Stove emissions in the field are frequently different than lab results in terms of $PM_{2.5}$ mass, but whether this difference also reflects a change in composition has implications for design and implementation of future intervention studies. Going forward, this knowledge will aid in understanding the relationship between changing domestic energy sources and human health outcomes.

10DU.6

An Investigation of the Optical Properties of Particulate Matter Emitted by Residential Biomass Hydronic Heaters.

JAKE LINDBERG, Patricia Fritz, Nicole Vitillo, Brian P. Frank, David Guerrieri, Marilyn Wurth, Gil H. LaDuke, Shida Tang, Thomas Wainman, Nathan Walz, Todd Crawford, *New York State Dept. of Health*

Combustion from commercial scale and residential heating contributes to ambient Particulate Matter (PM) pollution. Interest in the use of fuels such as wood, pellet, and chips for hot water heating in home and businesses is increasing because it can be domestically sourced, and is viewed as sustainable fuel options. We conducted a laboratory study of the flue exhaust from biomass-fueled water heating appliances using a 7-wavelength aethalometer (Magee AE33), a 3-wavelength aethalometer (Brechtel TAP), and a nephelometer (Thermo pDR-1500) to measure the relative emission of black carbon (BC) and Brown Carbon (BrC) emitted from these appliances under different operating (firing) conditions. Differences in the optical properties of ambient PM have been used as a tool to apportion PM contributions from wood combustion. During a combustion cycle we measured a wide range of Delta-C and angstrom exponent values which indicate BC and BrC emission are highly dependent on boiler operating conditions. The data we collected show that light-scattering measurements of woodsmoke particulate matter can be misleading when used as a metric of combustion efficiency without accounting for differences across burn-phase conditions.

10HA.1

Chemical Analysis and DTT Assay of Powder Form of Atmospheric Particles Collected by Cyclone. YOSHIHIRO TERUI, Daiki Shishido, Aoi Kanemaru, Tsubomi Sato, Tomoaki Okuda, *Keio University*

Numerous epidemiological studies have shown adverse health effects by fine and coarse aerosol particles such as PM2.5 and yellow sand. For this reason, aerosol cell exposure studies are currently required. However, cell exposure studies have some problems when we use aerosol particles collected by a filter sampling. For example, it is difficult to collect sufficient amount of aerosol particles for exposure, influence of contaminants derived from filter is inevitable at the time of exposure and operation to obtain particles from filter is complicated. Therefore, in this study we developed a high-volume sampler using virtual impactor and cyclone techniques for collecting aerosol in powder form without using a filter. This sampler can collect about 100 mg of coarse particles and fine particles separately in 2-3 weeks of operation. We collected fine and coarse aerosol particles at Keio University (in Yokohama) with this instrument. Chemical analysis of the collected particles has been carried out followed by DTT (Dithiothreitol) Assay to measure the oxidizing ability which is an indicator of the in-vivo oxidative stress of aerosol particles.

10HA.2

Aerosolization and Characterization of Cellulose Nanomaterials. BON KI KU, M. Eileen Birch, G.J. Deye, *Centers for Disease Control and Prevention, NIOSH*

Cellulose nanomaterials (CN) are emerging materials of interest for the forestry, paper, and pulp industry. The various forms, including cellulose nanofibers (CNF), micro fibrillated cellulose, and cellulose nanocrystals (CNC), can be produced from wood pulp and other biomass. While potential applications for these promising nanomaterials are emerging, particularly in the fields of sustainable materials and nanocomposites, the health and safety aspects of these varied products have not been fully studied, mainly due to the lack of relevant exposure data for workers. Microscopy analyses are useful for characterization of morphology and structure of CN, but they are not quantitative, and other methods have not been established/evaluated for monitoring worker exposure to these materials. Thus, method development, for both sampling and measurement, is needed to fill this knowledge gap. As part of this research effort, it is important to investigate a variety of bulk CN, including the CNC form, to determine: 1) the potential for aerosolization, 2) particle residence time in air, and 3) particle size distributions of the generated aerosols. We are, therefore, in the process of characterizing a number of CN to assess these properties. In this study, we investigated the aerodynamic characteristics of aerosolized CN powders.

Aerosols from bulk CN (i.e., CNC form, provided by Forest Products Laboratory, Madison, WI) are being generated in a controlled manner, to produce target concentrations and examine particle size distributions. Dry dispersion of CNC bulk powders is accomplished using an acoustic generator (AG) [Ku and Birch, 2015] and/or a vortex shaking technique (Ku et al., 2013). Airborne particle properties such as mobility and aerodynamic diameters were measured using mobility particle and aerodynamic particle sizers, and particle morphology was examined using optical or electron microscopy.

Preliminary results showed that aerosolized CNC particles have aerodynamic size distributions with a geometric mean diameter of about 1.5 µm and size range up to about 8 µm. In addition, the CNC particles were found to have a geometric mean mobility diameter of about 450 nm. The results indicate that the potential for aerosolization and a long residence time in air are expected to be high, calling for further characterization and development of reliable monitoring methods for these materials.

Acknowledgments

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10HA.3

Inflammatory Effects of Fine Aerosols Generated from Rapid Concrete Failure. LUPITA MONTOYA, Harish Gadde, Wyatt Champion, Ning Li, Mija Hubler, *University of Colorado Boulder*

Engineered materials in the built environment can deteriorate and fracture into particle shapes and sizes that may cause negative health effects in the wake of natural and man-made disasters, like the attack on the World Trade Center (WTC). Two and a half years after the attack, responders still experienced respiratory symptoms and pulmonary function effects. Similarly, ten years after the attack, excesses in total and specific cancers were reported in both responders and civilians exposed to WTC aerosols. Elemental analysis of these aerosols indicated that the main components were construction materials such as cement, concrete aggregate, ceiling tiles, and wallboard. Aerosol generated during concrete demolition have long been classified as an occupational health hazard for construction workers, reflected in OSHA's Crystalline Silica Rule: Construction. The primary risk comes from the inhalation of particles by workers; however, these particles can spread widely and pose an exposure risk to the public and the environment.

Results from our team showed that the aerosol size distributions generated by rapid fragmentation of concrete follow a bi-modal distribution tied to microstructural features of the concrete mix. This behavior is well described by introducing additional length scales in Gilvarry's derivation of the Rosin-Rammler-Sperlin-Bennet (RRSB) distribution. On this basis, we proposed that no new fragmentation theory is needed to describe aerosol particles if concrete fragmentation is regarded a composite material explicitly considering microstructural features, which create stress concentration at the microscale. By identifying a direct link between microstructural features and aerosol distributions, we proposed that it is possible to design concrete microstructures to limit aerosol exposure during dynamic failures such as structural collapse.

Reinforcing concrete with steel fibers has gained popularity in the construction industry as a composite material because it improves ductility of the concrete and distributes cracking. Recent work determined that multiple failure mechanisms act in composite materials to create macro-scale particle sizes and sub-micron aerosols by controlling the type of inclusion added to the concrete.

In this experimental study, cylindrical specimens of concrete mixtures containing steel fibers of different sizes were prepared and tested in a closed environment. Six types of concrete mixes were used to create 8 in x4 in test cylinders; 35 cylinders of each mix (total of 210) were made. Three fiber lengths (1, 1.5, and 2 in) as well as two inclusion percentages (0.6% and 0.8%) were chosen for this study. Dynamic compression tests were conducted on the cylinders at a constant displacement rate to simulate an extreme loading event. The generated fine aerosols (i.e., particulate matter ≤ 2.5 um in diameter, PM2.5) were collected during and after the failure. Aqueous extracts from these samples were then evaluated for pro-inflammatory effects (tumor necrosis factor alpha, TNF-alpha) using a RAW 264.7 murine cell line. Preliminary results of this study show that introducing fibers of any length or mass fraction increased the TNF-alpha response, compared to the control.

10HA.4

The Particle Size Distribution Measurements of Aerosol Generated by Common Inhalers and Nebulisers. ONDREJ MISIK, Frantisek Lizal, Miloslav Belka, Jakub Elcner, Jan Jedelsky, Jan Tuhovcak, Miroslav Jicha, *Brno University of Technology*

The important factor which influences the effect of inhalation treatment is the location of particle deposition in lungs, which directly depends on the size distribution of inhaled particles. [1]

Our aim was to compare various commonly available inhalers using an Aerodynamic Particle Sizer and match the results with data reported by manufacturers or with data acquired by different measurements.

The measurement

An Aerodynamic Particle Sizer (APS, TSI 3321, TSI Inc., Shoreview, MN, USA) was used for the measurement. A Fine Particle Fraction (FPF) was evaluated from the acquired particle size distribution. FPF represents the particles within the size range of 1–5 µm, which corresponds to the particles depositing well in lungs. As a second characteristics of the generated particle the count median of aerodynamic diameter (CMAD) has been used. [2]

The aerosol was sucked to the APS using an isokinetic probe and a conductive tubing. Special effort was made to arrange continuous sampling during the measurement of MDIs (metered dose inhalers), however, the manual triggering of the inhalers caused inaccuracies. [2]

Seven devices were measured (InnoSpire® Elegace®, Philips Respironics; Atrovent®, Respimat® SMI Placebo®, Respimat® SMI Spiolto®, Boehringer Ingelheim; Ultibro® Breezhaler®, Novartis; ANORO® Ellipta®, Glaxosmithcline; Brimica® Genuair®, AstraZeneca). In case of measurement of DPIs (dry powder inhalers) it was necessary to simulate patient's inspiration by a breathing simulator. In this case, the assembly was extremely sensitive to leaks. The leaks would cause an improper simulation of a breathing cycle, and hence a loss of precision. [2]

Results and discussion

Several interesting phenomena have been observed on the basis of the acquired data. In case of the nebuliser (InnoSpire® Elegance®, Philips Respironics®, USA) the measured CMAD increased during the measurement, which probably indicates coagulation of particles. The device operated for approximately 2.5 minutes and within this time the value of FPF increased from 60 % to 85 %. The FPF reported by the manufacturer is about 77 % and recommended time for the usage is 6 – 8 minutes. The results obtained for Atrovent® MDI generally correspond to the data measured by Mitchel et al. [3] on the Aerosizer [2]. In case of Respimat, the range for FPF reported by manufacturer should be between 65 – 80 %. Both of measured Respimat formulations fell into this interval. [2] The results acquired with APS generally agree with data reported by manufacturers or with data from measurements reported in literature. The inaccuracies and differences were most likely caused by weaknesses of assembly or by manual operating of the devices. During MDI measurements, the main source of problems was high velocity of the emitted aerosol, in DPI the proper actuation of devices using the breathing simulator. [2]

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10HA.5

Characterization of Airborne Fibrous Particle Deposition on Screens with Different Configurations. BON KI KU, G.J. Deye, *Centers for Disease Control and Prevention, NIOSH*

Understanding transport characteristics of workplace aerosol particles is important in assessing their fate in the respiratory system of workers who are potentially exposed to nanomaterials such as cellulose nanomaterials. In this context, inhalation of airborne nanomaterials and their deposition in the respiratory system is getting more attention during the process-related workers' activities in the workplace because it may cause toxicological responses. In order to estimate the toxicity of fibrous particles as a function of length, it is required to separate fibers by length and understand mechanisms related to fiber separation for use in toxicology studies. For nonspherical particles with high aspect ratios, such as aerosolized fibers and cellulose nanomaterials in the workplace, their deposition can be very different from spherical particles. In this study, we used screens with different mesh sizes to characterize deposition of fibrous particles on them and measured screen collection efficiency of fibrous particles as a function of aerodynamic diameter to better understand the deposition of the fibrous particles. Three screen configurations [i) without a laminar flow entrance length, ii) with the laminar flow entrance length (about 23 cm), and iii) centrally blocked screen] were tested to investigate the effect of screen pore size (10, 20, and 60 µm) and screen configuration on collection efficiency of fibers. Screen collection efficiency was obtained based on measurements of upstream and downstream concentrations of a test chamber either without or with a screen.

Test material was glass fiber powder used as a surrogate of asbestos, supplied by the Japan Fibrous Material Research Association (JFMRA) (Kohyama et al., 1997). This same material has been used in our recent studies for aerosolization of airborne fibers (Ku et al., 2013), fiber alignment in electric field (Ku et al., 2018) and classification of airborne fibers by length using screens (Ku et al., 2014).

The results showed that screen collection efficiency increases as screen mesh size decreases from 60 to 10 µm for both cases with and without entrance lengths. For the screen configuration without entrance length, higher collection efficiency was obtained than the case with entrance length probably due to increased impaction or self-filtration caused by the close proximity of inlet to screen. In addition, the difference between the collection efficiencies for the different configurations was small in the aerodynamic size range below 3 µm while it increased in the size range from 3 to about 7 µm, indicating that as large aerodynamic diameter is associated with longer fibers, some differential selection of fibers is possible.

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10HA.6

A Pilot Study of Air Quality in Puerto Rico after Hurricane María. NIRMALA THOMAS, Leonardo Calderón, Shahnaz Alimokhtari-V, Samuel Barreto Rios, Benjamin Bolaños-Rosero, Carlos M. Rodríguez-Minguela, Mayra Roubert, Clifford Weisel, Brian Buckley, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

Hurricane María is considered the deadliest storm of the hyperactive 2017 Atlantic hurricane season and one of the most intense tropical cyclones worldwide in the last year. It hit Puerto Rico (PR) as a strong Category 4 hurricane causing catastrophic damage across the Island.

In the aftermath of the hurricane, there were potential risks for increased exposures to emissions from diesel generators and microbial pollutants, as a result of the collapse of the Island's power grid and the severe water damage endured to buildings and housing structures. A rapid environmental response team from Rutgers University (New Jersey, USA) collaborated with University of Puerto Rico (Medical Sciences Campus and Mayagüez, PR) and Ponce Health Science University (PR) to evaluate the impact of the hurricane's landfall on biological and non-biological air quality parameters in PR and potential risk to human health.

A total of 10 sites consisting of 7 outdoor and 3 indoor locations were investigated in December of 2017 from San Juan to Ponce, PR. Among them, two EPA air quality-monitoring sites were used as references to compare the current air quality parameters with historical data. Biological and non-biological aerosol concentrations (mass concentrations of $PM_{2.5}$ and particle number concentrations of 0.3-10µm and >10µm), volatile organic compounds, and various gases (e.g., CO_2, CO, NO_2, O_3, and NO_2) were measured. Additionally, a passive bioaerosol sampler (Rutgers Electrostatic Passive Sampler, or REPS) and several low-cost particulate matter sensors (Air Visual) collected data for approximately two weeks.

Total outdoor mold concentration (#/m^3) ranged from less than 10^3 to $3x10^4$ and was dominated by allergenic Ascospores and Basidiospores species. Indoor sites showed elevated total mold concentrations of up to $8x10^4$ #/m^3 including toxin-producing Aspergillus and Cladosporium species, with no significant difference in the total concentration between outdoor and indoor sites ($p>0.05$). Indoor and outdoor sites registered both culturable bacteria and mold concentrations above 4881 #/m^3 (saturation level). The SidePak personal aerosol monitor (TSI, Inc.) detected $PM_{2.5}$ mass concentrations of up to 84 µg/m^3 indoors and up to 72 µg/m^3 outdoors. Two of the Air Visuals and the SidePak monitor at one of the outdoor sites located in southeastern PR also showed similar $PM_{2.5}$ levels. REPS captured biological particles using a ferroelectric polymer film (PVDF) and the post-sampling eluted liquid (40 mL) had concentrations of up to $5x10^6$ biological particles/mL.

These results suggest high concentrations of both biological and non-biological aerosols in certain local communities leading to health concerns. Future studies will address PR air quality and the resulting health effects in more detail.

10HA.7

Comparison of PAHs Levels and Health Risks in China, India and the United States. FENGLIN HAN, Jie Zhang, Qi Ying, Jianlin Hu, Sri Kota, Hongliang Zhang, *Louisiana State University*

Polycyclic aromatic hydrocarbons (PAHs) in the environment are of significant concern due to their high toxicity and adverse health effects. This study compares the concentrations of PAHs levels and health risks in three major countries, China, India and the United State (U.S.). Gridded anthropogenic emissions for China and India are generated from Emission Database for Global Atmospheric Research (EDGAR) version 4.3, and PAH emissions are from the global high-resolution PKU-FUEL-2007 inventory. U.S. emissions are generated using the Sparse Matrix Operator Kernel Emission (SMOKE) model version 3.7 and national emission inventory (NEI) 2011. Open biomass burning emissions are from the Fire Inventory from NCAR (FINN). A modified version of the Community Multiscale Air Quality (CMAQ) model (v5.0.1) was used to simulate the emissions, reactions, transport, deposition of 16 priority PAHs for obtaining the concentrations of PAHs species in gas and particulate phases. The PAHs concentrations of January, April, July and October in 2011, 2013 and 2015 were studied in the U.S, China and India, respectively. The source apportionment of PAHs is conducted using the brute-force and variations of source contributions are analyzed. The health risks, specifically excess cancer risk, of PAHs due to inhalation exposure of outdoor naphthalene (NAPH) and seven larger carcinogenic PAHs (cPAHs) are then estimated and compared in the three countries.

10HA.8

Pollution Characteristics and Health Risk Assessment of Heavy Metals in Particulate Matter in Changchun, Northeast China. LI NA, Sun Siyue, Han Weizheng, Kang Chunyu, *Jilin Jianzhu University, China*

In order to study the risk to human health caused by the concentrations of different particulate matter and the heavy metals attached to it in JingYue area in Changchun City. Samples of PM1 were collected by MVS sampler (German), PM2.5、PM5、PM10 and TSP were collected by medium flow sampler（Qingdao）at the top of civil engineering building of Jilin Jianzhu University from April to June in 2017.The concentrations of 8 heavy metals (Pb, Cd, Cr, Ni, V, Co, Sb, Mn) and Al were determined by ICP-OES, enrichment factor method was used to determine the enrichment degree of eight heavy metals, the health risk assessment models from USEPA was further used to evaluate the health risk of the population.The results showed that the concentrations of particulate matter exceeded the standard in different degrees, and the heavy metals of Cd and Pb exceeded the relative standards in all sizes of particulate matter, the concentration of Sb is obviously higher than that of other heavy metals. Enrichment factor analysis showed that the 8 heavy metals were enriched, among them, Cd, Pb and Sb were enriched extremely serious, EF values were between 102 and 105, EF values of Co and Cr were between 102 and 103, EF of Mn, Ni and V were less than 100. The HQ values of Cd, Cr, Ni, V, Mn and Sb, were respectively less than 1, indicating the non-carcinogenic risk may be acceptable. The R values of Pb, Cd, Cr and Ni were less than 10-6, indicating the carcinogenic risk was acceptable. Risk values from ingestion exposure pathway were higher than those of skin exposure and respiratory inhalation.

10HA.9

Physico-Chemical Characterization of Particles and Volatile Organic Compounds Emitted by Electronic Cigarettes and Heat-Not-Burn Products, Compared to a Reference Tobacco Cigarette. ARI SETYAN, Tobias Bührer, Florence Leuzinger, Woranan Netkueakul, Michael Patrick, Jing Wang, *ETH Zürich / Empa, Switzerland*

The electronic cigarette (e-cigarette) is a battery-powered nicotine delivery system. This device provides nicotine by inhalation into the respiratory system following the vaporization of an e-liquid, constituted of nicotine and flavors diluted in a solvent. Presented as a safer alternative to conventional tobacco cigarette, e-cigarettes have gained popularity worldwide over the past 10 years. More recently, a range of new products, in which tobacco is heated instead of burnt, were introduced into the market by several manufacturers. Intensive research is currently ongoing to assess the impact of these new products on air quality and human health, and thus to help policy makers to introduce regulations on their use in indoor environments.

In this study, we measured the concentration, chemical composition and size distribution of particles, as well as volatile organic compounds, in the mainstream emissions of a selected list of e-cigarettes (Puritane) and heat-not-burn tobacco products (iQOS, Ploom Tech), compared to those from a reference conventional tobacco cigarette (3R4F). The particle number concentrations and size distributions were measured with a fast mobility particle sizer (FMPS), while mass concentrations and size distributions were determined with a nano micro-orifice uniform-deposit impactor (Nano-MOUDI). Particles sampled with the Nano-MOUDI were also extracted with methanol, and analyzed by gas chromatography/mass spectrometry (GC/MS) to determine their chemical composition. Finally, volatile organic compounds (VOCs) were sampled with adsorbing cartridges (Tenax TA, Carboxen 569), and analyzed by thermal desorption-gas chromatography/mass spectrometry (TD-GC/MS), while the total hydrocarbon concentration was measured with a flame ionization detector (FID).

During each puff, the particle number concentration was approximately the same for all the products, between $1 \cdot 10^6$ and $2 \cdot 10^6$ #/cm^3. Particles emitted by all the products were totally dominated by submicron particles. However, those emitted by the conventional cigarette were slightly larger than those from the Puritane and iQOS (mode at 220 nm for 3R4F, vs. 150 nm for Puritane and iQOS), while the size distribution of particles emitted by the Ploom Tech was very broad, ranging from 10 to 200 nm. VOCs concentrations were 6 times higher with the conventional cigarette than with the Puritane and iQOS, and more than 100 times higher than with Ploom Tech. A wide range of mono-aromatic (mainly benzene- and furan-derivatives) and oxygenated compounds were identified in gaseous emissions of the conventional cigarette. Most of these compounds were also present in the iQOS, but in much lower concentrations, while VOCs emitted by the Puritane were mainly constituted of oxygenated compounds and alkanes. Toxicological and air quality studies are still needed to determine whether these new products really reduce risks for users and bystanders.

10HA.10

Aerosol Characterization of High-powered Electronic Nicotine Delivery Systems (ENDS). SUVAJYOTI GUHA, Seyed Ahmad Reza Dibaji, Samanthi Wickramasekara, Berk Oktem, Matthew R. Myers, *U.S. Food and Drug Administration, CDRH*

The use of electronic cigarettes, referred to here as ENDS (electronic nicotine delivery systems), has continued to grow in the last ten years. There is limited published data on the physical and chemical characterization of the latest fourth generation ENDS. These devices can supply up to 300 Watts (W) of power, compared with the 1-10 W range of previous generations. Furthermore, the heating coils aerosolize the e-liquid by direct contact, and have been reported to reach high temperatures (around 300 – 400 degree Celcius). Such high temperatures can break down e-liquids (including the carrier liquids propylene glycol (PG) and vegetable glycerin (VG)), yielding substantial amounts of aldehydes and acrolein, which can produce serious health effects.

The objective of this study is two-fold. The first is to investigate the mechanism of the aerosol formation in the latest ENDS by using multiple orthogonal characterization techniques with different temporal resolutions. The second is to investigate the impact of the high coil temperatures, as well as the PG/VG concentrations on the aerosol particle size, and its chemical constituents (both organic and inorganic). Our preliminary results suggest that fourth generation ENDS produce aerosols containing particles with multimodal size distributions that range from a few nanometers to several micrometers. Temporal resolution also appears to strongly influence the modes that can be detected.

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10HA.11

Characterization of Spray Aerosols Generated from Particle-Free Solutions and Nano-Particle Containing Suspensions (Nanoaers). LARS HILLEMANN, Paul Bergelt, Frank Bierkandt, Sandra Wagener, Jutta Tentschert, Emilia Visileanu, Hannes Hinterbichler, Helfried Steiner, Günther Brenn, Felipe Goni de Cerio, Joseph D. Brain, Michael Stintz, *Technische Universität Dresden*

Engineered nano materials (ENM) have a wide range of uses as additives in sprays (e.g. cosmetics, cleaning products, and coatings). The application of sprays generates an overspray, which may be inhaled by the user. The health risks of the inhaled aerosol depend on the particle size, but also on the composition of the aerosol. Small particles, including those in the nanometer size range, can reach deeper regions of the respiratory system. In turn, the aerosol particle size distribution depends on the parameters of the spraying process and the properties of the atomized fluid. Therefore, when the atomized fluid contains ENM, we want to know, if the aerosol contains particles of ENM in the nanometer size range, will there be a toxic effect in the respiratory system.

For this project, a test chamber was built to spray ENM containing suspensions onto an impaction plate and to measure the particle size distribution of the overspray at defined breathing distances. Eventually, lung cells will be exposed to the overspray in the further course of the project.

A spray can for customized applications was used for the spraying, which generates droplets in the size range similar to commercially available products.

The ENMs selected are nano-Ag, which is used for its bacterial inhibiting properties (e.g. in cosmetics or textiles), and CeO2, which is often added to lacquers and wood preservatives to improve their UV stability. CeO2 nanoparticles belong to the group of respirable granular bio-durable particles. Both materials are dispersed separately in solutions containing ultra-pure water, ethanol, TEA, HCl, MEK and Silanes in different compositions. Because of the strong dependence of the aerosol size distribution on the liquid properties, a test series was performed using the described setup with particle-free solutions, starting with ultra-pure water, and gradually adding components of the desired solution. Formulations with particles will show when any component generates measurable dried particles in the nanometer size range in the overspray.

This contribution is an important first step in this project. It describes the size distribution of droplets and dried particles released by the used spray can for different suspensions and solutions.

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10HA.12

Characterization of Heterogeneous Oxidation Products of Polycyclic Aromatic Hydrocarbons Using Online Mass Spectrometry. JAMES ROWE, Christopher Lim, Jesse Kroll, *MIT*

Polycyclic aromatic hydrocarbons (PAHs) are abundant environmental pollutants that can be toxic, mutagenic, and/or carcinogenic. These compounds are susceptible to oxidation in the atmosphere; this can affect their impact on human health, since oxidation processes will degrade the parent PAH molecule, but can also form secondary functionalized products that are potentially more toxic than the parent. Since most PAHs spend a large fraction of their atmospheric lifetimes in the particle phase, the identification of heterogeneous oxidation products is imperative for the understanding how atmospheric exposure might affect the health risk of PAHs. In this study, we simulated the heterogeneous reaction of PAH particles in the laboratory by exposing PAH-containing particles to gas-phase hydroxyl radicals (OH) within a flow tube reactor. PAH compounds were condensed onto ammonium sulfate seed particles and passed through the flow tube under conditions equivalent to ~1 week of atmospheric exposure to OH. The effluent was then analyzed using a suite of aerosol instruments, including an Aerosol Mass Spectrometer (AMS) and a Scanning Mobility Particle Sizer (SMPS). Together these measurements enable the characterization of product compounds, providing insight into potential reaction mechanisms and offering targets for future studies of the chemistry and health impacts of atmospheric PAHs.

10HA.16

Flavors, Nicotine, E-Liquid Composition and Coil Temperature Impacts Size Distribution of Electronic Cigarette-Emitted Particles. ARIANE LECHASSEUR, Simon Altmejd, Nathalie Turgeon, David Brunet, Caroline Duchaine, Mathieu Morissette, *Quebec Heart and Lung Institute - Université Laval*

RATIONALE. Electronic cigarette (e-cigarette) has become greatly popular throughout the years. E-cigarettes use propylene glycol and glycerol to deliver nicotine and flavors to the lungs. With hundreds of brands of e-cigarettes and thousands of types of flavors, characterization of the health impacts of e-cigarette is getting increasingly difficult.

OBJECTIVES. To investigate the impact of 1) coil temperature; 2) propylene glycol and glycerol concentrations; 3) nicotine presence and 4) flavors presence and type on e-cigarette particle size distribution.

METHODS. The inExpose e-cigarette extension (SCIREQ) was used in this study. We used the power-controlled and the temperature-controlled settings on the e-cigarette. Several e-liquids were used, using different propylene glycol and glycerol concentration. E-liquids contained 0 or 18 mg/ml of nicotine. For flavored e-liquids, menthol, vanillin and maltol were added. First, the e-cigarette was warmed up by puffing outside the collection system. Then, five 70 ml puffs, emitted every 30 seconds, were collected in a 45 L dilution chamber, with a dilution flow of 40 L/min. Measurements of particle size distribution were carried out by a Scanning Mobility Particle Sizer spectrometer (SMPS 3080, TSI Inc).

RESULTS. To assess the impact of different atomizer temperature, we first used the power-controlled function, using two different coil resistance. We showed that, for each resistance, an increase in power generated a greater number of large particles. We also used the temperature-controlled setting, and showed that higher temperatures generated smaller particles compared to lower temperatures. We then assessed the impact of propylene glycol and glycerol on particle size and found that an increase in glycerol concentration led to the generation of larger particles. As for flavors, we showed that despite minor effect of menthol and maltol, vanillin dramatically shifts particle size distribution towards larger particles. We finally demonstrated that, regardless of propylene glycol:glycerol ratio or the presence of flavors, the addition of nicotine increased the size of generated particles.

CONCLUSION. This study shows that coil temperature, propylene glycol and glycerol concentrations and presence of nicotine and flavors affects the size distribution of e-cigarette emitted particles. This in turn affects the lung deposition of such particles. Therefore, as much in the clinical as in the animal models, e-cigarette settings and e-liquid composition should be taken in consideration when investigating the pulmonary impacts of e-cigarette.

10HA.18

A Study of Aerosol Concentration and Composition on Cardiovascular Illness at a Semi Urban Site in Delhi. NISAR ALI BAIG, Mohammad Yawar, Kashish Jain, Sagnik Dey, Sandeep Singh, Deepti Kailath, Gazala Habib, *IIT-DELHI*

Many epidemiological studies have shown that ambient and personal concentration of both fine and ultrafine aerosol in urban environment are related to adverse cardiovascular effect, increased case of heart rate variability (HRV). We investigated the effect of aerosol and its components on the root mean square of successive differences (RMSSD) and standard deviation of normal-to-normal intervals (SDNN) and low to high frequency ratio (LF/HF) and ST segment depression/elevation. Sampling has been done at road site near the Main gate of IIT-DELHI, HAUZ KHAS, NEW DELHI during July 2017 to December 2017. The Electrocardiograph of healthy security guards stationed at main gate was recorded for 5-6 hours. The mass of aerosol was collected using SKC multi-stage cascade impactor for mass, and real time BC was monitored using aethalometer. The quartz filters were used to determination of EC (elemental carbon), and OC (organic carbon). Concentrations of $PM_{2.5}$ range from 208 to 547 $\mu g/m^3$ and black carbon ranged from 2.0-40.3 $\mu g/m^3$. These concentrations were significantly higher than those reported for developed countries. Therefore, we expect that the link between HRV parameters (i. e. indicator of arrhythmia), $PM_{2.5}$ and BC to be entirely different than those reported for developed countries. The statistical link between $PM_{2.5}$, BC and HRV will be discussed.

10HA.20

Laboratory Investigation of Oxidation Products from Ozonolysis of Electronic Nicotine Delivery Systems (ENDS) Emissions. CLAIRE FORTENBERRY, Michelle Molina, Walton Sumner, Brent Williams, *Washington University in St. Louis*

Electronic Nicotine Delivery Systems (ENDS) have become increasingly popular alternatives to traditional cigarettes since they were first marketed in 2004 [1]. Popular perception and recent literature suggest that ENDS are less harmful to users and bystanders than conventional cigarettes due to reduced production of typical combustion products [2]. These perceptions are likely to increase indoor use, as endorsed by many vendors [1]. However, indoor use will increase reactions of ENDS emissions with indoor oxidants such as ozone during and after ENDS use. Reactive constituents in ENDS emissions include aldehydes, glycol, tobacco-specific nitrosamines (TSNAs), and silicates [3], and vary with the nearly 8000 reported flavors available for purchase [4]. Furthermore, toxicant concentrations can vary due to the multitude of available ENDS designs. Additionally, ENDS emissions may, like cigarette smoke [5], deposit on indoor surfaces, oxidize, and resuspend, thereby contributing to indoor particulate matter (PM). Indoor oxidants therefore could affect first, second, and third-hand exposures related to ENDS emissions. These exposures have not been characterized.

We present results from laboratory studies to characterize the effects of indoor ozone oxidation on ENDS particles and gases. A Thermal desorption Aerosol Gas Chromatograph (TAG), which pairs automated sampling with gas chromatography-mass spectrometry analysis at hourly time resolution [6], was used to collect and analyze particle- and gas-phase emissions from ENDS devices. Many TAG systems feature collection of particles via inertial impaction onto a collection and thermal desorption (CTD) cell. We have modified our TAG system to include a temperature-controlled gas collector installed in parallel with the traditional CTD cell, which can collect material as volatile as formic acid.

The emissions of an ENDS device were introduced into a Potential Aerosol Mass oxidative flow reactor to investigate the effects of ozone exposure. We present the chemical speciation of gas- and particle-phase material from three popular e-liquid flavors and evaluate changes in abundances of key compounds with oxidation conditions.

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10IM.1

Using Comsol Multiphysics as a Tool to Predict Aerosol Deposition Spot Size of an Electrostatic Precipitator (ESP).

CALLE PREGER, Robert T Hallberg, Martin H Magnusson, *Lund University*

Aerosol technology provides an efficient means of producing engineered nanoparticles with controlled size and compositions, deposited on arbitrary substrates using an electrostatic precipitator (ESP). For some applications, it is important to achieve precise control of the nanoparticle concentration on the substrate. The motivation for this work is partly to design a better ESP, and partly to test how well a simple model, run on a modern standard PC, can mimic actual nanoparticle behavior.

In this work, COMSOL Multiphysics was used to simulate deposition patterns of nanoparticles and to predict the deposition spot size of an ESP for varying gas flow (0.2–2.2 lpm), particle diameter (5–100 nm), deposition voltage (1–10 kV) and the height between aerosol inlet and substrate (5–40 mm). A simple relation based on these calculations has been obtained based on a cylindrical 2D model of the deposition chamber, while a full 3D model was used to test the validity of the simulation as well as to predict the exact shape of the spot. The model predictions were validated with electron microscopy by measuring the spot diameter based on the surface coverage as well as by 2D profiling of the concentration on the substrate. This study shows the possibilities of using a commercial available product to predict complex aerosol physics. It also validates a model to use when predicting the deposition spot size for an ESP.

10IM.2

Evaluation of an Improved CPMA-Electrometer Reference Mass System in Measuring Black Carbon Particles. JOEL CORBIN, Alireza Moallemi, Jason S. Olfert, Fengshan Liu, Kevin Thomson, Gregory Smallwood, Prem Lobo, *National Research Council Canada*

For the calibration of instruments which measure the mass concentration of airborne particulate matter (PM), a traceable and sensitive reference system for mass concentration measurements is required. The CPMA-electrometer reference mass system (CERMS) satisfies these requirements, and has been demonstrated to perform reliably with low-volatility-organic as well as black-carbon aerosols, down to 5 μg m^{-3} concentrations (Dickau et al., 2015). This lower limit of detection (LOD) is satisfactory in the context of emissions testing, but only moderately so in the context of atmospheric pollution monitoring, where minimum of 1 μg m^{-3} is desirable.

The combined relative uncertainty of the CERMS has been previously reported as 4% (Dickau et al., 2015), but this relative value does not describe the LOD (an absolute value). Previous work has identified sources of uncertainty stemming from flow-meter imprecision, CPMA setpoint imprecision, CPMA setpoint bias, electrometer imprecision, and electrometer bias. Of these factors, the electrometer-bias uncertainty (resulting from baseline drift) is the only absolute value, and therefore becomes more important at lower concentrations; i.e., at the LOD. Here, we will systematically quantify and evaluate this uncertainty in terms of the Allan variance of the CERMS signal and corresponding baseline, for a system with an upgraded electrometer relative to the prior work. The utility of the upgraded CERMS will then be demonstrated using the calibration of an Artium LII 300 in High-Sensitivity mode, which is capable of detecting black carbon (BC) concentrations to levels of 0.2 μg m^{-3} and below.

10IM.3

Ozone and Absorbing Aerosol Measurements by Ultraviolet Total Ozone Unit (TOU) of FY-3A/B/C. HOUMAO WANG, *National Space Science Center, Chinese Academy of Sciences*

Total ozone unit (TOU) is one of the main payloads on FY-3A/B/C satellites and the first instrument for daily global coverage of total ozone monitoring in China. They have been in-orbit for almost nine years from May 2008. Total ozone is retrieved by ultraviolet radiance to observe global ozone distribution and its variation. Then, the absorbing aerosol index (AAI) is retrieved using 331 nm and 360 nm in 2013. It is used for atmospheric pollution observation of China, such as smog, dust storm, and biomass burning etc. In this paper, the quality and application of TOU data is shown and discussed, which includes L1B radiance, total zone, and AAI. Besides, the studying direction of future instruments is discussed.

10IM.4

Aerosol Deposition in the Sampling Train of PM CEMS. Yu-Mei Kuo, Shi-Bo Wang, Chih-Wei Lin, Sheng-Hsiu Huang, Hsien-Shiow Tsai, CHIH-CHIEH CHEN, *National Taiwan University*

There are several PM CEMS currently commercially available. From the standpoint of aerosol sampling, the performance of PM CEMS might be plagued with aerosol deposition in the sampling train, this potential and significant defect of PM CEMS has never been addressed before. The aims of this study were to evaluate the particle deposition in the sampling train and to improve the sampling efficiency.

In aerosol penetration test apparatus, an ultrasonic atomizer was used to generate micro-meter-sized challenging NaCl particles. The aerosol output was then introduced into the test chamber through a radioactive source, 10 mCi Am-241, to neutralize aerosols to the Boltzmann charge equilibrium, before diluted with filtered dried air. An Aerodynamic Particle Sizer was employed to measure the aerosol size distributions and number concentrations upstream and downstream of the sampling probe. The PM CEMS sampling train could be divided into three parts: sampling inlet with an elbow or goose-neck, connecting straight tube, and elbow adaptor connecting to TEOM or beta-gauge. The experimental data were then compared with the empirical models of particle deposition in bends of circular cross section and gravitational deposition of particles from laminar flows in channels. For a particular type of PM CEMS, the inner diameter of the sampling tube was 10 mm and the sampling flow rate was 2.1 L/min. The goose-neck sampling inlet was composed of a 120° bend tube followed by a 30° bend tube. The length of the straight sampling tube was 192 cm and the elbow tube had a 90° bend. The air velocity ranging from 10 to 100 cm/sec was employed to study the velocity dependency.

The loss of particle loss in the typical sampling train was found to be significant. The elbow or goose neck design resulted in over 10% aerosol deposition of 10 μm. The 192 mm long straight tube also caused over 10% deposition loss. The connecting elbow adaptor caused 20% deposition loss because of higher velocity. The overall loss of 10 μm particles was up to 40%, while the 2.5 μm particles experienced 5% loss. The experimental data showed higher aerosol deposition loss than the modelled ones. The discrepancy between the experiment and model was mainly on the inertial impaction loss in the elbow. That means the effect of curvature-diameter ratio of the elbow on the deposition loss needs to be further studied. Other factors such as elastic properties of the particle and the elbow tube, the roughness might contribute to the bounce-off and make the deposition loss unstable and unpredictable.

The currently commercially available PM CEMS sampling trains were designed to follow the isokinetic protocol, but did not consider the aerosol deposition loss in the sampling train due to gravitational settling and inertial impaction. The aerosol size separator with cut-point of 1.0 μm is highly recommended because of deposition loss due to gravitational settling and inertial impaction is less than 1%. The deposition loss is less than 5% if the 2.5 μm pre-separator is used. If the pre-separator is adopted for 1.0 or 2.5 μm, the isokinetic sampling criteria might become not that critical.

10IM.5

Performance Comparison of Field Portable Instruments to the Scanning Mobility Particle Sizer Using Monodispersed and Polydispersed Sodium Chloride Aerosols. EVANLY VO, Matthew Horvatin, Ziqing Zhuang, *NIOSH*

The aims of this study were to 1) evaluate the performance of portable aerosol instruments, including the handheld condensation particle counter (CPC), the portable aerosol mobility spectrometer (PAMS), the optical particle sizer (OPS), and NanoScan scanning mobility particle sizer (NanoScan SMPS), regarding their utility for evaluating respirator protection in nanotechnology workplaces and 2) to compare the measurements made with the handheld CPC, PAMS, OPS, and NanoScan SMPS with those measured with the reference SMPS.

Performance was evaluated in terms of particle concentration and particle size distributions using monodispersed and polydispersed NaCl aerosols. Monodispersed aerosols were controlled at the approximate concentration of 1x105 particles/cm3. Four monodispersed particle sizes of 30, 60, 100, and 300 nm were selected and classified for the monodispersed aerosol test. Three different steady-state concentration levels (low, medium, and high: approximately 8x103, 5x104, and 1x105 particles/cm3, respectively) were selected for the polydispersed aerosol test. Particle concentration and size distributions measured with the portable aerosol instruments were compared with those measured with the reference SMPS. For all four monodispersed aerosol sizes, particle concentrations measured with the NanoScan SMPS were within 13% of those measured with the reference SMPS. Particle concentrations measured with the PAMS were within 25% of those measured with the reference SMPS. Concentrations measured with the handheld CPC were within 30% of those measured with the reference SMPS. For the polydispersed aerosols, the particle sizes and concentrations measured with the NanoScan OPS compared most favorably with those measured with the reference SMPS for the three concentration levels of low, medium, and high (concentration deviations ≤ 10% for all three concentration levels; deviations of particle size ≤ 4%). Although the particle size comparability between the PAMS and the reference SMPS was quite reasonable with the deviations within 10%, the polydispersed particle concentrations measured with the PAMS were within 36% of those measured with the reference SMPS.

While further studies are needed to determine how to wear and operate these portable instruments under simulated workplace conditions or in a real working environment, this study provided the advantages and limitations of each portable instrument and therefore results from this study can be used, with appropriate caution, when selecting a suitable portable instrument for aerosol particle measurement in nanotechnology workplaces.

10IM.6

Aerosol Metrology for Atmospheric Science and Air Quality: The AEROMET Project. PAUL QUINCEY, Konstantina Vasilatou, Alfred Wiedensohler, Stefan Seeger, Luca Boarino, Petr Klapetek, Kai Dirscherl, Francisco Moreno, Peter Pedersen, Thomas Pedersen, Matjaz Zitnik, Jeanne Malet, Jenny Rissler, Szabina Torok, Markus Fiebig, Maria Ochsenkuehn-Petropoulou, Luca Stabile, Michele Laus, Armin Gross, Burkhard Beckhoff, *NPL*

The AEROMET project (2017 – 2020), within the European EMPIR programme, has the overall aim of developing and demonstrating methods for traceability and calibration of different aerosol instruments, with emphasis on environmental regulatory measurement. The relevant particle size range is from several nm up to 10 µm, mass concentrations (0.1 µg/m^3 to 1000 µg/m^3), number concentrations up to 10^6 particles per cm^3 and airborne particle composition for such components as metals, anions, cations, elemental carbon and organic carbon. The specific objectives of the project are:

To develop reproducible reference methods for PM$_{10}$ and PM$_{2.5}$, including the design and building of a demonstration aerosol chamber system – for calibrating instruments using representative generated aerosols and to achieve target uncertainties below 15 %.

To establish traceable validated methods for the determination of major components of particulate matter such as elemental and organic carbon (EC/OC), total carbon, anions and cations and major metals (e.g. arsenic, cadmium, mercury, nickel), in order to meet the data quality objectives of current regulation.

To develop calibration procedures for Mobility Particle Size Spectrometers (MPSS) for ambient measurements in the size range up to 1000 nm – in support of standardisation requirements from ISO TC 24 WG 12 and CEN TC 264 WG 32. In addition, to provide calibration facilities for measuring particle number concentration using Condensation Particle Counters (CPCs) in ambient air – as required by the technical specification EN/TS 16976.

To apply mobile x-ray spectroscopy techniques combined within particle sampling techniques to quantify particle compositions in the field in real time.

To qualify a synchrotron-based Grazing Incidence X-Ray Fluorescence (GIXRF) setup as a traceable reference for quantitative chemical aerosol analysis using mobile and bench top GIXRF instrumentation. Full traceability will be achieved by the use of fabricated micro and nanostructures.

The presentation will aim to summarize the goals and challenges of the project, which is currently in its early stages, in order to encourage contributions from the community.

10IM.7

Aerosol Charge Conditioning and the Characterization of a New Soft X-ray Charger. FREDERIK WEIS, Mara Pfeffinger, Maximilian Weiss, *Palas GmbH*

Prerequisite for the measurement of particle size distributions of an aerosol by differential mobility analyzer systems (DMAS) is the establishment of a known charge distribution. Soft X-ray chargers can offer an alternative to traditionally used radioactive neutralizers, which suffer from strict legislative handling and operation regulations. In this work, a new soft X-ray charger was developed and the performance was evaluated in comparison to a radioactive 85Kr source and with respect to the ongoing development of ISO standard 19996. Different aerosol generators were used to produce liquid and solid test aerosols with different pre-charge levels, as well as ambient air monitoring was investigated. In order to evaluate the aerosol charge distribution a new DEMC control unit incorporating two high voltage modules (positive and negative) was developed. By using two identical classifier columns and condensation particle counters the differences in the charged aerosol fractions can be directly monitored and characterized. The results will be discussed in comparisons to the bipolar diffusion theory and known particle charge distributions of other soft x-ray chargers.

10IM.8

Use of Mobile Air Quality Measurements to Investigate Highly Spatially Resolved Particulate Matter Concentrations in Houston. BLAKE ACTKINSON, Henry Wallace, Robert Griffin, Katie Moore, Ramon Alvarez, Grace Lewis, Elena Craft, Kyle Messier, David Miller, Joshua Apte, *Rice University*

Recent work has elucidated the capability of mobile air quality measurements to map air pollution concentration profiles on fine (<100s meters) spatial scales. Here, we evaluate the efficacy of using Google Street-View cars as a means of determining fine spatial profiles of pollutants in Houston. In addition to a suite of trace gas measurements, data collected includes mass concentrations of black carbon and total fine aerosol ($PM_{2.5}$) and number concentrations of ultrafine particles (UFP).

The Google Street-View cars were deployed from July 2017 through March 2018 across 35 different Houston census tract polygons representing a range of geographic locations, emission sources, air quality monitor deployment, and socioeconomic status of residents. Median values of mean air pollutant concentrations were mapped in 30-meter segments throughout the cars' drive paths. In addition, to identifying the influence from point sources such as cement batch plants, metal recyclers, and oil and gas operations, data collected were compared to fixed monitor data to investigate the representativeness of the fixed monitoring data. The collected data also were used to estimate the background pollutant concentrations spatially and to investigate the temporal nature of the fine-scale pollutant maps (weekend versus weekday, mid-day versus early morning or evening). Future work will incorporate these data into analyses on air pollution health effects.

10IM.9

Using a Differential Mobility Analyzer and an Electrostatic Precipitator in Tandem for Determining Physicochemical Properties of Airborne Particles. SPYRIDON BEZANTAKOS, Maria Katergi, George Biskos, *The Cyprus Institute, Nicosia, Cyprus*

Tandem differential mobility analyzer systems (TDMAs) are commonly employed for determining some of the key physicochemical properties of aerosols such as hygroscopicity and volatility. TDMAs are, however, bulky and costly, limiting their employability in cases that require high mobility and/or concurrent spatially distributed measurements. To address these limitations we have developed and tested a cylindrical precipitator which can be used as a replacement of the second DMA in TDMA systems. This approach, namely the tandem DMA-precipitator (TDMA-P), reduces significantly the bulkiness complexity and cost of a tandem system, since the precipitator is compact and does not require a sheath flow and consequently all the necessary peripherals for controlling it. Its classification zone (approx. 8cm in our design) consists of a central metallic rod, on which high voltage (HV) is applied. This rod is concentrically placed within a metallic cylinder that is always grounded. Penetration of charged particles through the cylindrical precipitator is dictated by the applied HV on its central electrode and the sample flow rate. Measurements of the relative penetration (i.e., the penetration of particles when the central electrode is at HV divided by their penetration when the central electrode is at 0V) of the sampled particles is related to their size at a specific and constant sample flow rate.

A tandem system consisting of a DMA (for selecting monodisperse particles), the cylindrical metallic precipitator and a condensation particle counter (CPC), was used for measuring the relative penetration of monodisperse ammonium sulfate (AS) particles, sizing from 10 to 400 nm through the precipitator at voltages varying from 5 to 1400 V, and at flow rates of 0.3 and 1.5 lpm. The measured relative penetration curves could be thereafter used for calculating the apparent electrical mobility diameter of an unknown aerosol population, providing information on its size. The performance of the TDMA-P was characterized using laboratory-generated ammonium sulfate particles, and the system is currently being deployed in the field.

10IM.10

Validation and Calibration of Particle Sizers with Test Aerosols. TORSTEN TRITSCHER, Thomas Krinke, Andrea Tiwari, Juergen Spielvogel, Francisco Romay, Stephan Große, Andreas Rudolph, Oliver F. Bischof, *TSI GmbH*

The validity of data obtained with particle counters and sizers depends on their accurate calibration against a known standard that typically is provided by the manufacturer. However, normal use of an instrument may affect the calibration over time, for instance through contamination or drift of sensors controlling the device. The recommended time interval for calibration and the complexity of the calibration procedure may vary from instrument to instrument. For this reason, the user's validation of the instrument performance against the specifications is an important contribution towards assuring long-term measurement consistency.

Globally, several NMIs (National Meteorological Institutes) or standard-setting organizations regulate or recommend test aerosols and complete calibration procedures. We introduce methods to generate aerosols with known properties in the size range of a few nanometers to several micrometers. Here we focus on aerosol generators that can provide aerosol particles fulfilling criteria required for the validation of counters as well as sub- and super-micron sizers without a complex setup. The methods are easy to use and can be conducted by the user.

The aerosol properties need to be adapted to the spectrometer that needs to be verified. Important properties are an adjustable size range and concentration output, monodispersity, output stability, aerosol composition, and handling of the generator including practical aspects of the generator design, such as portability or changing solutions. We introduce and compare the performance of two generators with different test aerosols from the liquid phase.

Portable atomizer aerosol generators like the TSI Model 3079 provide aerosols with particle size distributions in the sub-micrometer size range. A drawback is that they produce very high aerosol concentrations usually above 10^7 particles/cm^3 that require subsequent dilution. The size of the particle mode diameter ranges from 50-200 nm, depending on the oil or salt concentration. A novel Portable Test Aerosol Generator (TSI Model 3073) is introduced that works with a submerged Laskin nozzle to generate the initial droplets. It allows flow and concentration adjustment (flow rate: 0.3 to 4.5 L/min, concentration range 10^5 to $>10^7$ particles/cm^3). For operation in the field it can be equipped with a battery pack. The long-term stability and the reproducibility of the aerosol generation has been investigate by measuring the variation of the size distribution over time with a Scanning Mobility Particle Sizer (SMPS). Typical particle materials from solution (sodium chloride, NaCl), liquid (oil) and suspension (Poly-Styrene Latex, PSL) have been studied.

The validation of spectrometers for the micrometer size range, like Optical Particle Counter (OPC) or the Aerodynamic Particle Sizer (APS) require the generation of particles in the size range between 3 is ideal for the validation. The Flow-Focusing Monodisperse Aerosol Generator (FMAG, Model 1520) is a lab-based instrument that produces highly monodisperse aerosol mainly in the supermicron size range. This ability makes the FMAG a valuable tool for verifying the performance of supermicron sizing instruments. The particle size can be adjusted very accurately in the range from 0.7 to 15 µm. We have investigated the high monodispersity and reproducibility for different aerosols and will show our results for particles from solution (NaCl), a liquid (glycerol) and a suspension (PSL). The particle size distributions have been measured by an APS Spectrometer (TSI Model 3321). The dispersion of biological particles such as cells or spores is possible with this generator as well and preliminary results will be shown.

We will present data and instrument specifications detailing the suitability of these two generators for use as on-site validation tools for aerosol sizers and counters.

10IM.11

Application of New Butanol-based CPCs to City Air Monitoring and Comparative Instrument Characterization. Andrea Tiwari, Jacob Scheckman, Aaron Avenido, Juergen Spielvogel, AXEL ZERRATH, *TSI Incorporated*

Introduction

The new Condensation Particle Counters (TSI model series 375x) have been applied to suburban air quality measurements in winter 2017/18 for further characterization and comparison to other established particle technologies.

Sampling was conducted through a rooftop environmental sampling system with PM10 sampling inlet and a multiple port flow splitter. Environmental data is available from an on-site weather station feeding data into a publicly accessible weather network.

The station is located in a mixed residential and light-industrial area and is close to freight railroad tracks, a railroad junction and an interstate highway, all located within one mile of the sampling location.

The collected data was reviewed with two goals in mind:

1. Observation of ambient air quality using a suite of instruments including the standard submicron sizer (SMPS), two supermicron sizers (APS, OPS) and real-time quartz-crystal microbalance MOUDI impactor (QCM-MOUDI). Particle size, number concentrations, mass concentrations, and mass distributions were all assessed.
2. Inter-comparison of particle counters; the set of three counters included two working fluids (water and butanol) as well as two cutpoints (2.5 and 7 nm).

Results

Ambient air observations:

- Particle number concentrations: Particle concentrations range from less than 5,000 #/cm³ to up to more than 100,000 #/cm³, depending on wind direction and time of the day, and the activities of local particle sources. This concentration range is typical for city air, and can now be measured accurately using CPC Model 3750, which has an upper concentration limit of 100,000 #/cm³, 10-fold higher than its predecessor. In addition to the upper concentration limit, the cutpoint size of the 3750 CPC – 7 nm – is also appropriate for conducting ambient sampling. Ambient sampling in Europe is governed by the CEN standard (CEN/TS 16796), which specifies that CPCs should have 50% counting efficiency at 7 nm. This cutpoint size is also relevant to ambient sampling in the US, where near-road monitoring frequently uses a 7 nm cutpoint CPC.
- Particle size distributions: The size distribution data recorded with an SMPS scanning from 11 to 478 nm, shows that the majority of particles is <100 nm (ultrafine particle fraction), with occasional events showing up to 200 nm sized particles. Since SMPS data provides insight into changes in particle size with time, it can be a useful supplement to CPC data in that it can suggest changes in particle sources.

Inter-comparison of several particle counters:

- Sampling under stable conditions (average temperatures around -6 °C, low wind speed and wind direction mostly from NW) resulted in agreement between two different CPC models to better than 1%. The two models in question had different cutpoints – model 3750 at 7 nm and 3752 at 4 nm – which indicates that the vast majority of ambient particles were larger than 7 nm. The wind direction points to the aerosol being dominated by traffic, with influence from the nearby highway.
- Sampling under transient conditions (characterized by a wind direction change from west to southeast) resulted in agreement between two CPCs of the same cutpoint specification to within 1% with low scatter (r^2 of 0.94). These two Ultrafine CPCs measured approx. 9% higher number concentrations than the Standard CPC (model 3750 with 7 nm), suggesting that some particles in the ambient air were < 7 nm.

The observations described above support the laboratory instrument characterization results; data from both settings will be presented.

10IM.12

Methods to Minimize Diffusion Losses for sub-3nm SMPS Measurements. JACOB SCHECKMAN, Modi Chen, Hee-Siew Han, Juergen Spielvogel, *TSI Incorporated*

Scanning Mobility Particle Sizer (SMPS) systems employing a Differential Mobility Analyzer (DMA) for sizing and a Condensation Particle Counter (CPC) for counting are widely used for measurement of aerosol particle size distributions. Such measurements of particles as small as 1nm in diameter are needed in academia and industry for applications including nucleation and growth, engineered nanoparticle synthesis, reaction kinetics and combustion research. Diethylene glycol (DEG) has been used as a working fluid to grow sub-2.5nm particles to a size detectable with a butanol-based CPC, thus enabling SMPS size distributions in this size range. A 1nm SMPS system employing a DEG-based Nano Enhancer along with a butanol-based CPC has been commercially available from TSI since early 2016.

As particle size decreases, diffusion loss rates increase dramatically. Less than 10% of 20nm particles are lost in a 1 L/min laminar flow through a straight 3m tube. For the same conditions, the loss rate of 2nm particles is nearly 95%, and greater than 99% at 1.5nm. Further, because of the size-dependent nature of diffusion losses, the mode of a monodisperse (σ_g=1.15) size distribution shifts from 1.5nm entering the 3m tube to 1.8nm on exit. Although diffusion losses can be corrected for, below 2nm the required correction factor can be several hundred or higher for a typical SMPS system. To minimize uncertainty due to counting statistics, care must be taken (minimize unnecessary tubing lengths, use transport flows, etc.) to configure the SMPS system to maximize particle penetration.

Here we present a compact SMPS setup for the TSI 1nm SMPS system. The components are assembled with the neutralizer coupled directly to the DMA, which is installed directly onto the Nano Enhancer inlet. This configuration eliminates Electrostatic Classifier internal plumbing, and neutralizer-to-DMA and DMA-to-CPC transport tubing. This configuration maximizes particle penetration through the system and minimizes uncertainties in the final corrected concentrations.

In addition, we derive a semi-empirical diffusion correction for the optimized, compact 1nm SMPS system configuration. For each system component, particle losses were measured experimentally under limited flow rate/particle size conditions. The straight-tube laminar flow loss equations were used to fit an “effective length” that is then used to calculate losses for other flow rates and particle sizes. We also present experimental validation of the correction at sizes <2nm, and evaluate its impact on real-world size distribution data generated by such a system.

10IM.13

Fourteen Orders of Magnitude of Organic Volatility in One Instrument: The Comprehensive Thermal Desorption Aerosol Gas Chromatograph (cTAG). REBECCA WERNIS, Nathan Kreisberg, Susanne Hering, Allen H. Goldstein, *University of California, Berkeley*

Aerosols are a source of great uncertainty in radiative forcing predictions and have poorly understood impacts on human health. Most aerosol mass is formed in the atmosphere from reactive gas phase organic precursors, forming secondary organic aerosol (SOA). Semi-volatile organic compounds (SVOCs) (effective saturation concentration, C*, of 10^{-1} to 10^{3} μg/m^{3}) comprise a large fraction of organic aerosol (OA), while intermediate volatility organic compounds (IVOCs) (C* of 10^{3} to 10^{6} μg/m^{3}) have been demonstrated to efficiently react to form SOA and to be abundant in the atmosphere. Volatile organic compounds (VOCs) ($C^* \geq 10^{6}$ μg/m^{3}) are also critical to measure precursors to SOA due to their even greater abundance and their reactivity, as well as their impacts on ozone formation.

Until now, no single instrument existed that is sensitive to compound-specific VOCs, IVOCs and SVOCs (C* 10^{-1} to 10^{9} μg/m^{3}). The Comprehensive Thermal Desorption Aerosol Gas Chromatograph (cTAG) can detect this full range of SOA-producing organic precursors and semi-volatile products. cTAG can obtain concentrations hourly and gas-particle partitioning for SVOCs bihourly, enabling observation of the chemical evolution of these species through oxidation and partitioning into the particle phase. Online derivatization for SVOCs measured by cTAG enables detection of polar and oxidized species in addition to non-polar ones, expanding speciated identification and quantification to a broader range of SOA compounds.

cTAG is a two channel instrument which measures concentrations of $C_5 – C_{16}$ alkane equivalent volatility VOCs and IVOCs on one channel and $C_{14} – C_{30}$ IVOCs and SVOCs on the other channel coupled to a single High-Resolution Time-of-Flight Mass Spectrometer (HR-TOF-MS) detector, thus achieving consistent quantification across 14 orders of magnitude of vapor pressure. The HR-TOF-MS enables detection limits below 1 ppt over the entire range as well as improved compound identification by assigning chemical formulas to exact mass ion measurements from continuously measured full mass spectra. Dual miniature gas chromatographs allow for use of two chromatography columns each optimized for the volatility range of its respective channel. The VOC/IVOC collector consists of a layered bed of adsorbent materials while the SVOC collector is a passivated metal mesh filter. Collectors are thermally desorbed and their contents injected onto the corresponding chromatography column and analyzed in series. Online derivatization on the SVOC channel is achieved by exposing the sample to derivatization agent-saturated helium during desorption. On line calibration systems tailored to each channel allow accurate quantification and identification confirmation for hundreds of compounds.

In this work we present the operating principle and design details of cTAG as well as data from a winter and spring field deployment in Livermore, California, a city which had multiple exceedances of the ozone and PM2.5 U.S. National Ambient Air Quality Standards over the last few years, placing it among the cities in the San Francisco Bay Area with the poorest air quality. In winter, wood burning for heat combined with reduced boundary layer mixing leads to elevated $PM_{2.5}$ levels. Regional contributions from the Bay Area and the San Joaquin Valley add to the local air pollution burden. Hourly concentrations of VOCs/IVOCs and SVOCs were obtained concurrent to routinely monitored VOCs and other criteria and regularly measured air pollutants at a collocated Bay Area Air Quality Management District monitoring site; the cTAG data are compared with these measurements as validation. Based on known chemical tracers and temporal correlations between measured compounds, we present the initial findings of VOC, IVOC and SVOC concentrations and partitioning to elucidate the relative contributions of pollution sources to $PM_{2.5}$ in Livermore.

10IM.14

Investigating Catalytic Stripper Based System for Measurement of Sub-23 nm Particles from Vehicle Engine Exhaust.

MOSTAFIZUR RAHMAN, Adam M Boies, *University of Cambridge*

The European Union (EU) has included Gasoline Direct Injection (GDI) vehicles and non-road machinery engine into its Solid Particle Number (SPN) based Euro-VI emission standard. Diesel vehicles are complying with the SPN based standards from 2011 mainly by integrating Diesel Particulate Filter (DPF) in the exhaust system. Thanks to Particle Measurement Program (PMP) which paved the pathway to implementing the SPN based standard. However, there has been a widespread debate about the exclusion of sub-23 nm particles and semi-volatiles from PMP measurement protocol. Some studies found a high concentration of sub-23 nm particles in post DPF emissions, where other concluded it resulted measurement artifacts. Recently, this debate has got new momentum after the inclusion GDI vehicles into SPN based standard and subsequent introduction of Gasoline Particulate Filter (GPF) into the GDI vehicle exhaust system. Studies reported the consistent presence of 10-20 nm mode particles in GDI engine exhaust which are either elemental carbon or semi-volatiles (SV). The PMP system is yet to prove its robustness while measuring the sub-23 nm particles. Therefore there is a requirement for an even more robust measurement system to include sub- 23 particles into emission standards.

A measurement system employing catalytic stripper (CS) could be a potential solution to this problem. CS system removes volatile and semi-volatile particles by evaporating them upon heating at 350°C and subsequent oxidation. Therefore it eliminates the possibility of renucleation of those semi volatiles upon cooling down of the gas stream. This study under PEMs4Nano project is investigating the robustness of CS based measurement system in measuring sub 23 particles. We are testing a range of catalytic strippers for their SV and solid particle penetration efficiencies. The results suggest almost zero SV penetration efficiency and 50-60% solid particle penetration efficiency for 10^4 #/cm^3 particles at 10 nm size. Further works are in progress to improve the solid particle penetration efficiency at 10 nm and beyond by optimizing the catalyst length, type, geometry and flow condition. Primary results of this study indicate that it is possible to reduce the cut-off point of SPN emissions from 23 nm to 10 nm, but a further comprehensive investigation is required to down size the cut point beyond 10 nm. The complete outcome of this project will help to implement 10 nm cut point in future EU emissions regulation.

10IM.15

Study on CPC Time Response – Modelling and Measurements. JOONAS ENROTH, Juha Kangasluoma, Frans Korhonen, Joonas Vanhanen, Michel Attoui, Tuukka Petäjä, *University of Helsinki*

Condensation particle counters (CPC) time response consist of multiple factors, such as the flow rates and instrument geometry. In practice, the measurement of the time response is complicated, and the results can easily be biased by an unfit measurement setup. Providing the ideal instantaneous step change in aerosol concentration, while using well defined aerosol composition and size range, and maintaining a stable concentration for extended time periods is in practice extremely difficult. This has led to numerous different approaches being used for response time measurements, for instance valves (Quant, 1992), differential mobility analyzers (Buzorius, 2001) and spark generators (Wang et al., 2002). Due to the aforementioned complexities, the problem lends itself well to modelling.

In this study we present a comparison of both modelled and measured time response results for the Airmodus A20 CPC. We also compare the impacts that individual processes play in determining the time response, i.e. influence of factors such as diffusional losses, particle growth and gravity, as well as the dependency on the test aerosol properties, such as the used particle size distribution. In addition, we present the measured time response data for numerous commercial CPC's. The results of this work aim to further the understanding of basic aerosol physics as it is applied to instrument development and performance.

10IM.16

Experimental and Theoretical Evaluation of Air-Microfluidic MEMS PM Sensing Technologies. IGOR PAPROTNY, Dorsa Fahimi, Omid Mahdavipour, Mandana Hajizadehmotlagh, *University of Illinois at Chicago*

Air-microfluidics encompasses the use of micro electro mechanical systems (MEMS) to develop low-cost/small footprint lab-on-a-chip devices for air quality monitoring. This poster reviews the recent advances in MEMS low-cost environmental sensors. In particular, we describe latest results from theoretical and experimental comparison between different implementations of gravimetric direct-read MEMS airborne particulate matter (PM) sensors developed in our lab. We show that the sensitivity ad stability of the sensor is fundamentally dependent on the design of the mass-sensing resonator, as well as the driving circuitry. We describe the figures of merit of this new and emerging technology, and show examples of successful implementation of this technology in several types of direct-reading PM mass sensors developed in our lab.

10LC.1

The Impact of Ambient Conditions on the Performance of a Low-cost Air Quality Sensor Package (Koala). XIAOTING LIU, Rohan Jayaratne, Phong Thai, Matthew Dunbabin, Lidia Morawska, *Queensland University of Technology*

Low-cost sensors have been widely used in environmental monitoring. With respect to air quality monitoring, the application of large numbers of low-cost sensors can implement the results of regulatory air quality monitoring. The flexibility of the low-cost sensors enables them to be installed to cover a wide proportion of the targeted area. In this study, the performance of a range of low-cost sensors was tested.

In this study, a low-cost sensors package equipped with a particulate mass (PM) and a carbon monoxide (CO) were developed, calibrated and tested by the Queensland University of Technology, Australia. They were installed at an established air quality monitoring station at a typical roadside location and operated in parallel with standard instruments such as a tapered element oscillating microbalance (TEOM) and a CO analyser for a continuous period of three weeks. Meteorological parameters such as temperature, relative humidity, wind speed and wind direction were also obtained from the air quality monitoring station. The PM and CO data acquired were compared with the data collected by the reference station.

Here, we present the results obtained on a typical 24-hour day of measurement – the 26th of July 2017, by one of the sensor packages. We observed that both PM and CO concentrations from the sensor package followed a similar trend, with the measured values from the reference station. Fairly good linear relationships (Pearson r = 0.80 for $PM_{2.5}$ and r=0.92 for CO) were also found between the sensor package and the reference instruments. The $PM_{2.5}$ concentrations from both reference station and sensor package showed high correlation coefficients (Pearson r = 0.72 for reference instrument and r=0.90 for sensor package) with relative humidity. The possible reason could be the temporal distribution of the $PM_{2.5}$ during this day had the same variation trend as the relative humidity which had a high value during the night time and low value during the day time. Meanwhile, the CO concentration from both reference station and sensor package had low correlation relationships (Pearson r = 0.48 for reference instrument and r=0.45 for sensor package) with relative humidity.

A limitation observed in this study is that the $PM_{2.5}$ sensor in the sensor packages underestimated the particle number concentration from motor vehicle emissions. This was because the lower detection limit of the low-cost PM sensors was 300 nm, which is significantly higher than the size of most of the vehicle emission particles. The CO concentration value shown by the sensor package was consistently lower than the value from the reference instrument. This showed that an offset value needs to be added to the observed readings in future applications. Analysis of more collected data from sensor packages and reference station need to be completed to have a better understanding of the performance of the low-cost air quality sensor package.

10LC.2

The National Plan of Environmental Internet of Things Using Widespread Air Quality Sensors in Taiwan. CHIA-PEI CHEN, Yeuh-Bin Wang, Fan-Lun Chen, Kun-Hsing Liu, Bo-Chieh Yang, Shuenn-Chin Chang, *Taiwan Environmental Protection Administration*

In Taiwan, how to effectively identify the pollution source location is an essential issue, especially when the residential and industrial areas are in close proximity. It requires a widespread monitoring network that was difficult to build in terms of the economic and technical feasibility until low-cost and portable air quality sensors and the Internet of things (IoT) emerge recently. TEPA (Taiwan Environmental Protection Administration) is dedicated to provide our citizens high-quality living environment and thus propose the concept of environmental IoT (EIoT) plan to assist the source identification and then the environmental enforcement. For testing the concept, TEPA implemented a small-scale EIoT project in a seaside industrial area and then learned the lessons of the sensor limitation in extreme environment, the local coordination issues on electricity and land use, maintenance issues, the sensor data processing, the appropriate deployment density setting, and the collaboration with law enforcement department. By the experience of the EIoT project, TEPA believed the EIoT is practicable and valuable and subsequently promoted a national EIoT plan involving more than 10,000 air quality sensors deployed island wide, incorporating the approaches of public and private sectors. TEPA also developed a sensor testing system by comparing the performance between the tested sensor and the high-quality monitoring station to confirm the sensor usability. TEPA anticipates that the innovative EIoT can enhance the performance of environmental enforcement to avoid illegal emission and provide the nearby environmental information for local habitants.

10LC.3

Design and Optimisation of Low-cost Air Quality Sensor Package (KOALA). XIAOTING LIU, Matthew Dunbabin, Bryce Christensen, Rohan Jayaratne, Phong Thai, Lidia Morawska, *Queensland University of Technology*

There is currently a large selection of low-cost air quality monitors available in the market for consideration, although it was determined to be unrealistic to test them all individually for the scope of this study given the diversity in the manufacturing quality, functionality and consistency of monitoring results. The aim of the study was to develop a modular sensor package which can reliably measure the air quality and individual pollutants within acceptable tolerances with consideration for the low-cost production costs of the devices. The processes for the design and optimisation of low cost air quality sensor packages will be demonstrated in this study.

This low-cost air quality sensor package (named KOALA), developed by QUT, was equipped with Plantower PM sensor PMS1003 and Alphasense CO-B4 sensor as well as temperature and humidity sensors. The Plantower PM sensor PMS1003 and Alphasense CO-B4 sensor were selected because of their consistent and reliable performances in our previous lab and field tests. The CO sensor was used to identify the combustion sources of air pollutants which was shown to be the main source for air pollutants in our study areas. With the combination of PM and CO sensor, the KOALA air quality sensor package was able to identify the difference between sources of air pollutants in the targeted area.

The KOALA air quality sensor package has been designed to be robust enough for remote field deployment and longevity, while still performing the required monitoring functions. The external components of the device include a custom designed hardened plastic casing, solar panel and mount, PM sensor intake, PM sensor fan exhaust, CO sensor rain guard, and the mounting plate for the device. Considerations were made for water resistance in the design of any external components, with all devices having silicone applied around external components before deployment.

The internal structure of the KOALA includes a programmable Arduino board, 3G Module, Antenna, microSD card, power switch, battery, CO sensor and Plantower PM Sensor. With the function of solar panel and rechargeable battery, the KOALA air quality sensor package was able to operate in the outdoor environments without the need for a dedicated mains power source. The software was using the Arduino software framework.

The improvement and optimisation of the sensor package has been completed through a staged internal lab testing and then external deployment campaign. The following problems were encountered and subsequently resolved during the continuous testing and operation of the air sensor package. 1)Achieving low-power management for relatively high-power sensors (e.g. Plantower) which could cause unexpected restarting of the sensor node; 2) Data delivery delays due to low-signal 3G connectivity issues; 3) power management issues causing inability to send data, and the automated switching of the unit to caretaker mode to protect the battery pending charge; 4) Incorrect clock settings due to power loss on the internal board battery. To solve these problems, optimisation of both hardware and software of the sensor package was completed and involved: 1) custom software development to overcome the hardware power management issues: 2)to prevent the node batteries to drain completely before deployment which may cause trouble to get them charged again (Lithium batteries), major software change has been done with regard to power management;3) For locations with limited sunlight for the solar system during the day, software was developed; 4) increase the solar panel size; 5) developed a deployment protocol for ensuring solar energy harvesting and suitable 3G signal quality for data transfer.

Data communication from the sensors is performed using a variety of low bandwidth technologies. The data is stored on the sensors SD card, which retains records in a queue to upload at a nominal interval, currently each 30 minutes. The data adheres to the lightweight MQTT messaging format, a condensed string format to reduce overhead during transmission. Using 3G, the data is sent to an IoT endpoint on Amazon Web Services (AWS). It is then parsed through a variety of AWS services to reside in a PostGreSQL database, which is accessed via a public web interface.

The website to date has stored over 400,000 records successfully during this testing phase, which around 2% purged due to poor date and time data. The website offers dynamic graphing of the incoming sensor readings including battery health, PNC readings, PM readings, temperature, humidity and CO information. The raw data is available in table format, or as a downloadable JSON format. Additional features will include extendable querying of the dataset and CSV format downloads for larger datasets, and a geo-spatial visualisation in preparation for the expansion of the monitoring network and introduction of mobile sensors.

10LC.4

Evaluating Performance of Low-Cost Optical Particle Counters in Sensing Bioaerosols; an Experimental Chamber Study. PARICHEHR SALIMIFARD, Donghyun Rim, James Freihaut, *The Pennsylvania State University*

Recent rise of low-cost aerosol sensing technology has opened a new horizon in the study of particulate matter (PM) exposure with a broad range of applications; from establishing outdoor PM monitoring networks with high spatiotemporal resolutions; to integrating indoor PM sensors into building ventilation controls to mitigate PM exposure in occupied spaces. In order to reliably use low-cost sensors for any of the aforementioned applications, their performance under any of specific application conditions should be fully examined first. Various studies have conducted field and lab experiments to investigate the low-cost optical particle counters' (OPC) performance. The results showed a strong dependence of the tested low-cost OPCs on the particle characteristics and environment conditions. Although, it is evident that low-cost PM sensor performances could vary considerably when exposed to various particles, very little information about the performance of low-cost sensors in monitoring bioaerosols is available. Given the significance of bioaerosols in exposure studies and their associated adverse health effects, this study investigates the performance of low-cost optical sensors in detecting the common indoor bioaerosols.

To investigate the effects of particle characteristics and concentrations, PM sensor responses were examined under exposure to varying concentration levels of biological (dust mite, pollen, cat fur, and dog fur) and non-biological (monodisperse silica and melamine resin particles in 1 and 2.8 µm) aerosols. Each particle sample was dispersed into a chamber (76×76×42 cm) using a computer-controlled syringe injection system. Size-resolved particle number concentration was measured by four tested low-cost OPCs (Speck, Airviz Inc.; Dylos, Dylos; OPC N2, Alphasense; and IC Sentinel, Oberon Inc.) and the reference sensor (AeroTrak, TSI) simultaneously. Linear regression analysis was used to compare the sensor responses to that of the reference sensor.

Results showed different combined effects of aerosol size, optical characteristics, and concentration on the sensor response. Concentration has the most dominant effect on the linearity of the low-cost sensors. In lower particle number concentration ranges, low-cost PM sensors showed nonlinear response, whereas, in higher concentration ranges they exhibited high linearity. The dividing line between the nonlinear and linear concentration regions varied with the sensor and the tested non-biological aerosol type and size. The fairly homogenous response to the bioaerosols allowed for determining a dividing line (5/cm^3) between nonlinear and linear regions that is common amongst all the tested low-cost OPCs. This study findings imply that low-cost OPCs can be used in monitoring specific concentration ranges of bioaerosols, once they are calibrated prior to deployment.

10LC.5

Evaluation of the Performance of a Lightweight, 3D Printed SMPS. KONSTANTINOS BARMPOUNIS, Anne Maisser, George Biskos, *AK LemonLabs Ltd.*

Monitoring the quality of the air, and particularly the concentration and size of airborne particles, is increasingly important for assessing the impacts of air pollution on human health and climate. Most of the existing and commercially available instruments for measuring atmospheric aerosol particles are bulky and expensive, thereby limiting the density of the monitoring networks around the world. In order to circumvent these limitations many efforts have been made to develop mobile and lightweight instrument for aerosol measurements in the recent past. However, the vast majority of these efforts go at the expense of counting and/or sizing resolution, or require a lot of engineering efforts, and are thus very expensive.

The approach used here to develop a cost-effective nanoparticle monitoring holds great potential for revolutionizing the manufacturing of instruments. This is done by replacing heavy stainless steel parts by extremely lightweight plastic parts, coated with a graphite layer for conductivity. The method has been already introduced by Barmpounis et al. in 2016 and has been further developed since. The major advantage of using plastic pieces is that they are extremely inexpensive, very easy to manufacture, and enable reduction of weight by more than an order of magnitude.

Here we will present the results of a performance evaluation of an SMPS system consisting of a 3D printed Differential Mobility Analyzer (DMA) and a 3D printed Faraday Cage Electrometer (FCE). The dimensions of the DMA are identical to the instrument described by Barmpounis et al. The total weight of the instrument is only 3kg.

In order to confirm the robustness and reproducibility of the manufacturing technique we have built and tested 5 SMPS systems. The performances of the DMAS were evaluated in a tandem DMA system, where we used a homemade stainless steel DMA as a classifying DMA. The 3D printed DMAs were scanning over the entire size range. The FCE were tested using a Condensation Particle Counter and a commercial FCE in parallel.

In conclusion we found the 3D printed manufacturing technique to be appropriate for producing highly reproducible and robust instruments. This new manufacturing technology can largely contribute into the wider distribution of SMPS measurement devices leading into a tighter meshed network of monitoring stations on a global scale as a second step. In addition, such systems are suitable for use onboard of unmanned aerial vehicles (UAVs). More efforts are currently put into the development of a CPC using a similar approach to enable detection of low concentrations of particles, which is crucial for ambient measurements.

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10LC.6

Fluorescence Analysis of Combustion Particulate Matter on Solid State Substrate. GAURAV MAHAMUNI, Gregory Korshin, Igor Novosselov, *University of Washington*

Exposure to airborne particulate matter (PM) from dissimilar sources such as cigarette smoking, combustion engines, agricultural, and forest fires can contribute to cardiovascular and respiratory diseases. Spectroscopic analysis of PAH compounds present in PM is used for source apportionment of potentially harmful particles, but this involves cumbersome sample processing and requires expensive laboratory equipment. We present a novel PM analysis approach based on the use of solid-state Excitation Emission Matrix (EEM) measurements. The collection substrate is a glass coverslip coated with a layer of Polydimethylsiloxane (PDMS). PM of any provenance (e.g., cigarette smoke, wood smoke, and diesel exhaust) are collected on the substrate using electrostatic parallel plate collector. PM collection on reference filters is done in parallel to generate reference samples. Following the collection, the gravimetric analysis determines mass loading on the substrate and the filters. EEM of the sample on the PDMS substrate is obtained by direct excitation of the substrate. These solid-state measurements are compared with EEM from filter extraction into cyclohexane. Relevant experimental data shows that EEM data from PDMS substrates match well with EEM data in liquid extracts for typical PM sources. Limit of detection for combustion-generated PM can be calculated by correlating mass concentration and total fluorescence obtained using this method. The technique can be used to develop a compact, low-cost sensor for source apportionment of PM chemical composition.

10LC.7

Evaluation of Low-Cost Particle Sensors for Ambient Air Quality Monitoring. NUERAILI KUERBANJIANG, Meilu He, Suresh Dhaniyala, *Clarkson University*

In recent years, the use of low-cost particle sensors (LCPS) has become popular for air quality monitoring. Typically, these sensors are used in ambient monitoring after calibration against co-located FRM samplers. Such calibration efforts provide for site-specific conversion of sensor signals to PM. For a comprehensive understanding of the capabilities and limitations of these sensors, we conducted a series of tests with a range of popular OEM sensor units, and established the performance characteristics of the sensors under controlled conditions. We used size-classified particles from a differential mobility analyzer (DMA) and determined the concentration detection limit of LCPS for particles of varying compositions. The performance of the LCPS was established by comparison with number concentration measurements made using a condensation particle counter (CPC). The performance of the units was established as a function of temperature, humidity, and ambient wind-speed. We will present experimental results from our studies and identify sensor handling issues that are critical for accurate air quality measurements with these sensors.

10LC.8

AQ & U: A Layered Framework for Integrating Sensor Data of Variable Quality and for Engaging Citizens about PM2.5 Exposure. KERRY KELLY, Pierre-Emanuel Gaillardon, Miriah Meyer, Ross Whitaker, Anthony Butterfield, Pascal Goffin, Tom Becnel, Amir Biglari, Tofigh Sayahi, *University of Utah*

The emergence of commodity sensors is changing the way we think about and estimate our personal exposures to potentially harmful air-quality events. AQ & U is building a layered framework for integrating sensor data of variable quality using state-of-the-art data modeling and visualization coupled with a citizen-science effort to engage residents to host and maintain sensors across the city. The goal of AQ&U is to provide real-time, localized estimates of PM2.5 levels across the Salt Lake Valley - a region that periodically experiences some of the worst short-term $PM_{2.5}$ pollution episodes in the country. During the winter of 2017 the Salt Lake Valley had over 100 sensing nodes in the AQ&U network, and the network included high-quality data from state monitors and research-grade instrumentation as well as lower quality information from community networks of low-cost, $PM_{2.5}$ sensors. We performed laboratory and field calibration on a portion of the low-cost sensors, but the quality of the measurements from the existing network of community sensors was less certain. Sensor readings and uncertainty estimates for each sensor were used in a regression model to estimate $PM_{2.5}$ concentration at the neighborhood scale. Complexities, such as elevation and roadways, are being added to the model. Citizens can view the sensor data, estimates of $PM_{2.5}$ and uncertainty through engaging visualizations. AQ&U takes a citizen-centric approach both in the way that we deploy and maintain our sensor network, as well as in the way we design tools for public access. We rely on individual and school volunteers to host sensors and help identify poor-quality data. For students, we developed a hands-on teaching module that incorporates building blocks and simple electronics to build a light-scattering PM detector. This allows students to understand the operating principal of their sensor, making it less of a “black box”.

10LC.9

Ambient Air Quality and Carbon Monoxide Exposure Among School Children in Cap Haïtien, Haiti. AUDREY DANG, Eben Cross, Melissa Chapnick, Lora Iannotti, Joseph Steensma, Jay R. Turner, Brent Williams, *Washington University in St. Louis*

Few air quality measurements have been reported for the country of Haiti, limiting our understanding of the contribution of air quality to disparities in health endpoints. Solid fuel use for cooking by over 90% of Haitian households suggests significant chronic exposure to carbon monoxide and particulate matter (PM) [1]. Transportation emissions also contribute to poor air quality in urban and peri-urban areas. Recent advances in the design and calibration of lower-cost sensing platforms such as ARIsense provide the means to better understand ambient air quality and evaluate exposure in resource-challenged areas [2].

We will present ambient monitoring and personal exposure measurements from a broader study of chronic carbon monoxide exposure and health in Cap Haïtien, Haiti. Monitoring consists of lower-cost ARIsense integrated sensor packages (CO, CO_2, NO, NO_2+O_3, PM, relative humidity, temperature) deployed to two primary schools in urban and peri-urban neighborhoods. Stationary monitoring at the schools also includes quartz filter sample collection for offline organic speciation with a Filter Thermal Desorption Aerosol Gas Chromatograph (Filter TAG). Personal exposure to carbon monoxide among students at the schools is assessed with integrated passive dositube measurements as well as continuous measurements from low-cost electrochemical sensors. We evaluate ambient and personal measurements to investigate drivers of personal exposure.

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10LC.10

A Low-Cost Unipolar Charger for Charged Particle Measurements. MEILU HE, Suresh Dhaniyala, *Clarkson University*

Increasingly scientists are interested in mapping air quality at high resolution over large areas to accurately assess exposure to ambient particles. For such studies, a large number of low-cost particle sensors are required for large-area particle concentration monitoring. In response to such requirement, several low-cost sensors have been developed for particle concentration measurements. Almost all of these sensors operate on the basis of optical scattering, which means that particles smaller than ~ 300 nm cannot be detected by such sensors. The population of particles smaller than 300 nm often dominates ambient number concentration and possibly more important from a human health perspective. To detect these particles, we are developing a low-cost electrical-mobility based sensor, with particle concentrations measured by an electrometer. To boost sensor signal and detect particles under low concentrations, we developed a low-cost unipolar charger that is compact in size, and simple in design. Using a standard corona Tungsten wire and a compact HV, steady positive ions were generated and their concentration was measured. Additional electric field is applied to minimize particle contamination on the wire. Particle size dependent charging fractions were measured for the charger. We will present the design of the charger and its charging and transmission characteristics and some initial results of the integrated performance of the charger with the low-cost electrical-mobility sensor.

10LC.11

Indicating Black Carbon Exposure with a Smartphone App Using Image Analysis. Gang Chen, Mengxuan Cai, Bruce Urch, Frances Silverman, Yushan Su, ARTHUR W. H. CHAN, *University of Toronto*

Exposure to indoor air pollutants leads to 4.3 million premature deaths each year (World Health Organization, 2012), mostly in low and middle-income countries. Particulate matter (PM) is a pollutant of special concern, which contributes significantly to those deaths. As one of the major components of fine PM ($PM_{2.5}$) from combustion sources, black carbon (BC) has been suggested as a better indicator of harmful particulate substances than undifferentiated PM in studies of health effects, but current commercial BC sensors remain too costly to deploy widely. The objective of this project is therefore to develop an affordable and relatively accurate BC measurement method using a smartphone. Here we use image analysis to determine the amount of BC collected on a filter substrate. The image of the filter substrate is first obtained using a smartphone, and the darkness of the filter substrate is then determined by comparison to standardized colour panels. To obtain the relationship between the filter colour and BC mass, we have analyzed over 1300 filter samples collected across Ontario, Canada by the Synchronized Hybrid Ambient Real-time Particulate (SHARP) monitor with corresponding BC measurements. Results show a strong correlation (R^2>0.92) between BC loading (measured by commercial BC instruments, e.g. aethalometer) and the colour information (RGB) obtained from the image, demonstrating the feasibility of our method. We also verify this model with further sampling from engine exhaust and personal sampling in Toronto and China. The outcomes of this project will lead to a relatively accurate method to measure BC exposure at significantly lower costs compared to commercially available BC sensors and can be used to inform the general public in developing countries about BC exposures.

10LC.12

Evaluation of Wearable Low-Cost Particulate Matter Sensors. Ryan Chartier, JONATHAN THORNBURG, *RTI International*

Air pollution is one of the largest health risk factors in the world and exposure to poor air quality can lead to a multitude of adverse health outcomes. Local air quality is often measured by outdoor monitoring stations, but Americans spend greater than 90% of their lives indoors, making improved assessment of personal air quality exposures on a community and city level a top priority for health researchers. Reducing exposures to harmful indoor air pollutants, such as particulate matter (PM), will have positive health benefits, yet outside of small targeted research studies, real-time PM exposure data are rarely available at a highly spatially-resolved personal level.

The increasing availability of low-cost air quality sensors will make it possible to deploy large numbers of devices to collect highly spatially resolved personal level exposure data while increased computational power and innovative data analysis and visualization tools will allow us to understand exposure trends and hotspots at unprecedented resolution. However, low-cost air quality sensors generally provide poor data quality relative to more expensive reference monitors, limiting their appeal to exposure-health researchers.

We evaluated the performance of several commercially available wearable low-cost PM sensors against reference monitors including the RTI MicroPEM personal exposure monitor and a TSI DustTrak 8530. Three of each low-cost sensor were collocated with the reference monitors and challenged with various types of PM (black carbon, oleic acid, test dust) at concentrations ranging from approximately 0-500 $\mu g/m^3$. Each test was repeated multiple times, on different days, to assess measurement repeatability of the sensors. Key performance indicators (accuracy, precision, repeatability, data capture efficiency) for each sensor were quantified. Data aggregation and correction algorithms were developed to process and improve the data quality obtained from the low-cost sensors, and to support the visualization of exposure data as we move towards an integrated network of sensors.

10LC.13

Evaluating the Transferability of Low-Cost Sensor Calibration between Different Regions and Spatial and Temporal Variation in Air Quality in Hartford, CT. Kyle Terracciano, Fatema Parvez, Carl Malings, Rebecca Tanzer, R. Subramanian, KRISTINA WAGSTROM, *University of Connecticut*

One of the biggest challenges facing researchers hoping to deploy low-cost monitors is developing reliable calibration approaches for many of these technologies. Zimmerman et al. (2018) present a novel approach applying machine learning to calibrate the Real-time Affordable Multi-Pollutant (RAMP) sensor package for CO, NO_2, O_3, and SO_2. The RAMP uses electrochemical sensors for each of the gases. This calibration approach relies on data collected when monitors are collocated with reference monitors to develop a calibration model using random forests (RF). Each RAMP uses a PurpleAir or Met-One Neighborhood PM monitor for fine particulate mass ($PM_{2.5}$).

In this work, we evaluate the transferability of the calibration model developed in Pittsburgh, Pennsylvania for use in a different, but meteorologically similar, region - central Connecticut. It is imperative that we determine how well a calibration model developed in one area performs when moved to another region. For this test, we have selected two locations with fairly similar meteorology: southwestern Pennsylvania and central Connecticut. We will share the results of a three week collocation test in Hartford, CT using three RAMP monitors calibrated in Pittsburgh, PA using a random forest model hybridized with a multiple linear regression (MLR) model for higher concentrations. The RAMP data will be compared with data from a local regulatory monitoring station (maintained by the Connecticut Department of Energy and Environmental Protection) to determine the performance of the Pittsburgh calibration. We will also share the results of an additional three week study with the monitors distributed over three sites in a Central Connecticut, to examine spatial and temporal variability in air quality around Hartford.

10LC.14

Comparison Experiment of Low Cost Sensors for Aerosol and Gasses at Dem Athens. Prodromos Fetfatzis, Stergios Vratolis, Evangelia Diapouli, KONSTANTINOS ELEFTHERIADIS, *NCSR Demokritos, Athens, Greece*

Nowadays there is an intense development of low cost and small size environmental measurement systems for aerosol and gasses, using a variety of sensors for scientific experimental use and smart cities monitoring. Most of them are based on open source, common hardware platforms, such as ODIN, PACMAN, UPAS, mentioned at Olivares et.al (2015), Volckens et.al (2017), Wang Y. et al. (2015). They measure temperature, humidity, carbon dioxide, carbon monoxide, PM10, PM2.5, VOCs, etc. Nowadays new multiple low cost sensors appear in the market using new technologies from companies that construct sensor integrated circuits. All the low cost projects are aiming to sensor systems as cheap as possible without compromising reliability. An intense experiment is under way in order to compare and assess the level of accuracy-stability of low cost sensors that are now commercially available. This comparison experiment contains ambient air measurements in DEM station, generated aerosol and mixed gasses measurements at DEM Lab chamber. Light scattering particle sensors, such as the PPD42NS by Shinyei Inc., DSM501A by Samyoung Inc., GP2Y1010AU0F (Sharp Inc.), PMS Plantower series, etc. will be tested for the aerosol particulate matter. These sensors provide optical particle counting measurements for particles larger than 0.5 micrometers. CO2 and other gas sensors such as the EE893, and Alfasense will be compered. Instruments like SMPS, OPS that measure the aerosol size distribution from 25nm to 30µm, ERL's certified sensors and standard gasses will be used for the tests of the atmospheric parameters and gases sensors.

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10LC.15

Toward the Development of a Portable Single-Particle Fluorescence Spectrometer for Inexpensive Analysis of Bioparticles Collected on a Substrate. BENJAMIN E. SWANSON, Donald R. Huffman, J. Alex Huffman, *University of Denver, CO*

Bioaerosols, such as fungal spores, pollen, plant fragments, and bacteria, are present in all ecosystems and everywhere people live and work. They are linked to interesting environmental systems and are the cause of a variety of health effects, from seasonal allergies to airborne infections. In particular, allergenic effects caused by anemophilous (airborne) pollen torment huge fractions of the population and result in significant societal cost in terms of missed days of work and school. While daily weather forecasts now routinely include predictions of pollen levels, the direct measurements that support these predictions are most commonly accomplished through collection and optical microscopy performed by trained individuals. Much effort has been invested in the development of autonomous pollen counters over the last several decades, but these efforts have not yet produced small or inexpensive sensors capable of characterizing pollen with high reliability. In particular, many instruments utilized laser- or light-induced fluorescence (LIF) to interrogate particles. Real-time LIF instruments for bioaerosol detection are generally either costly to purchase (i.e. >$100k) or offer poor spectral resolution and poor discrimination ability.

Here we describe work toward the development of a handheld, portable instrument for the characterization of fluorescence spectra from many individual particles collected onto a substrate. The presentation will provide an overview of the properties of a benchtop version of instrument that was recently published [1]. The instrument utilizes four excitation sources (280 nm, 370 nm, 405 nm, and 450 nm) to probe a broad range of fluorophores and can collect fluorescence spectra from particles larger than approximately 0.5 µm in size. We showed the application of the first version of the instrument to four species of pollen [2], highlighting the ability to successfully separate pollen species using the K-means clustering algorithm.

We then applied the experience with the benchtop instrument to a prototype, handheld instrument (version 2) built using the same general principles. The smaller instrument (13 x 13 x 7.5 cm; 58 g) utilizes two excitation sources at a time and a Raspberry Pi camera as a detector, but collects the same information from each individual particle as version 1. Both instruments collect particle size and well-resolved fluorescence emission spectra (400 – 750 nm at ca. 2 nm resolution) for each excitation source. The small version was produced as a battery-powered aerosol detection system, as published [1]. Recent improvement in excitation sources used in the instrument have not yet been engineered to run on batteries, but this is planned. We will show an overview of the spectra collected by instrument version 2 and will demonstrate the ability of the instrument to differentiate between pollen species. The instrument is still in development, and at present an aerosol collection system is not yet coupled to the detection optics. Once a collection system is paired to the detector, we anticipate that a portable version of the spectrometer will represent a fundamental step forward in the ability to characterize pollen particles at a significantly lower cost than existing single-particle LIF spectrometers. We anticipate that it will also enable pollen or mold spore detection at higher spatial resolution than is currently available. The instrument was also designed as a tool for the investigation of particles and for education about fluorescence spectra by citizen scientists or schools.

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10LC.16

Open-source Aerosol Modelling: Electrical Charging and Transport with Applications in Low-cost Sensing. ROBERT NISHIDA, Nene Yamasaki, Adam M Boies, Simone Hochgreb, *University of Cambridge*

Electrical charging of particles and subsequent transport and electrical current measurement is used in a range of aerosol measurement devices including low-cost ultrafine particle sensors. Unipolar and bipolar diffusion chargers and photoelectric chargers yield predictable charge states necessary for correct measurement inversion to yield particle sizes and concentrations. However, each of the chargers are subject to localized flow and charging effects (de La Verpilliere, Swanson, & Boies, 2015; Nishida, Boies, & Hochgreb, 2017), which are neglected in simple zero-dimensional (0-D) charging models. In low-cost sensors, the integrated measured signal is a direct function of particle polydispersity and models often assume monodisperse particle distributions and low or high mean charge states to simplify the solution algorithm (Maisels, Jordan, & Fissan, 2002; Marra, Voetz, & Kiesling, 2010). Whereas these assumptions may be straightforward for simple systems, representing charge and diameter by a single variable may not be sufficient in other cases. Nevertheless, solving the flow and charge transfer calculations can quickly become cumbersome even for a small number of variables.

In this work, we present an open-source toolbox for generalized aerosol electrical charging and transport equations. The toolbox includes simple, 0-D models up to full, 3-D computational fluid dynamics (CFD) models. We solve the steady-state conservation equations for particle/ion charging and transport (convection, diffusion and electric field transport). The charging equations include unipolar diffusion, bipolar diffusion, and/or photoelectric charging. Sample cases are included for simple 0-D models which retain sufficient complexity in charging equations, but neglect localized geometrical effects. Source terms may be selected at run-time: for example, particle diffusion loss to walls. The solution algorithm is generalized to monodisperse or polydisperse particle distributions and up to 50+ particle charge states. The codes are written using C++ in OpenFOAM, an open-source CFD platform. By incorporating a CFD platform, the solution may be easily adapted to different flow conditions and geometries, and the code may be operated natively in parallel if needed. The computational method is verified by comparing with existing charging models and experimental data where possible (Nishida, Boies, & Hochgreb, 2018).

The modelling toolbox is used to investigate the effect of particle polydispersity in low-cost ultrafine particle sensors which charge particles with unipolar diffusion charging or photoelectric charging mechanisms. Low-cost devices are experimentally calibrated with controlled aerosol sources to provide metrics such as mean particle size and total concentration from one or more electrical current measurements. However, an aerosol with a large standard deviation in particle size will provide a significantly different signal from a monodisperse aerosol with the same mean particle size. Therefore, further understanding of the effect of polydispersity is required to improve the accuracy of low-cost sensors. We solve the conservation equations for particle/ion charging and transport (convection, diffusion and electrical transport) for a laminar, steady-state, incompressible flow. Lognormal particle size distributions are represented with upwards of 50+ coupled conservation equations for multiple size bins and charge levels. Modelling results show that the effect of polydispersity on integrated electrical current can be represented by a monodisperse distribution characterized by a surface-weighted (photoelectric charging) or length-weighted (unipolar diffusion charging) mean diameter and total concentration for a large range of particle distributions and operating conditions offering a convenient simplification to the conservation equations.

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10LC.18

Taking Ambient Air Monitoring to the Next Level - Multiple Applications with the Fidas® Technology for Fine and Ultrafine Particles Measurements. FREDERIK WEIS, Stefan Hogekamp, Leander Mölter, Maximilian Weiss, *Palas GmbH*

Air pollution due to particulate matter and the related negative effects (health problems, economic damages) has become one of the major problems our society is faced with today. In order to be able to investigate and to assess the real exposition of the general public in a comprehensive way, the performance of precise and accurate measurements of particulate matter is an essential part of air pollution control.

The Fidas® sensor applies the well-approved measurement technology of optical light scattering on single particles and is equipped with a polychromatic LED light source with long-term stable output. The scattered light intensity is detected under 90° through a patented aperture technology, thus preventing border-zone error and enabling for precise coincidence detection. The implemented approach allows for an easy field calibration as well as a permanent online-monitoring of the calibration status.

Due to its modular design, the Fidas® sensor technique has been adapted to specific devices to cover a large range of possible applications, which will be highlighted in this presentation. It includes regulatory monitoring of PM2.5 and PM10 in official networks by the type-approved and EN-/MCERTS-certified Fidas® 200, indoor and workplace measurements with the portable Fidas® FROG or due to the lightweight sensor technology also installations on flight robots or drones for assessment of line and area sources are possible. Results from the latest approval campaigns will be presented.

Since the Fidas® sensor delivers also total number concentration and particle size distributions with a high time resolution, this can be valuable for e.g. source appointment, prognosis models or the detection of condensation and droplet formation.

For the monitoring of ultrafine and engineered nanoparticles, the Fidas® is combined with an Universal-SMPS to measure from 8 nm to 40 µm to get a comprehensive picture of the air pollution. The overlapping region of the two systems can then be used for extended characterisation.

10LC.19

Using Low-Cost Particulate Matter Sensors to Monitor Photovoltaic Panel Soiling. SARAH TOTH, Michael Hannigan, Marina Vance, Michael Deceglie, Leonardo Micheli, Matthew Muller, *University of Colorado Boulder*

The deposition of ambient particulate matter (PM) onto the surfaces of photovoltaic (PV) modules can reduce power output by almost 50% in some locations [1]. Ongoing efforts to characterize this phenomenon, referred to as "natural soiling", have been primarily informed by existing EPA air monitoring stations that are often too geographically distant from the location of interest with respect to the known time scale of ambient PM deposition rates [2]. EPA monitoring stations also inform the sensitive public (i.e. the young, elderly, and asthmatic) of high-risk days due to PM. The goal of this study is to evaluate the efficacy of deploying low-cost PM sensors to inform the state of soiling in PV modules and to dictate cleaning schedules.

To achieve this goal, a low-cost, laser-based ambient PM sensor (DC1100 Pro, Dylos Corp.) has been calibrated and deployed along a PV soiling station consisting of a set of solar cells, one of that is cleaned daily and another that is not. This station was deployed along an air monitoring station managed by the Colorado Department of Environmental Health (CDPHE). The data is being continously collected and analyzed for accuracy with respect to the CDPHE station data and the potential for scaled-up deploymen. This work will allow PV cleaning maintenance to be informed by real-time, local data rather than the inefficient traditional regular intervals.

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10LC.20

Seasonal Concentrations of PM2.5 and PM10 in Borovoye, Kazakhstan Using Low-Cost and Well-Reference PM Monitors. MEHDI AMOUEI TORKMAHALLEH, Aigerim Jaxybayeva, Soudabeh Gorjinezhad, *Chemical and Aerosol Research Team, Nazarbayev University*

Kazakhstan is the first energy consumer and contributor to various fossil-fuel emissions in Central Asia. In 2014 the highest per capita household coal consumption occurred in Poland, followed by Kazakhstan. Coal combustion produces considerable amount of PM which will be responsible for acute and chronic health effects. A recent study estimated annually a minimum of 7500 premature deaths in Kazakhstan due to exposure to PM. Estimating the PM concentrations and the related health impact requires a proper sampling network. The analysis done by World Bank revealed that air quality monitoring network in Kazakhstan has many features that are out of date, and in many cases experiences unrepresentative sampling. The number of monitoring sites are low, and the selection of monitored pollutants does not comply with recognised priority pollutants. Thus, there is a crucial need for the establishment of a proper air pollution monitoring network in Kazakhstan. This study aims to investigate the summer and winter PM2.5 and PM10 concentrations in a rural area (Boroovye), 258 km north of the capital city, Astana in Kazakhstan. Two low cost monitors including Dylos and Speck has been utilized together with Dusttrak DRX, TSI. The low cost PM and the Duttrak DRX recorded the PM concentrations every minute and every thirty seconds, respectively. The summer sampling was conducted during July 2017 and the winter sampling will be performed during February 2018. The average PM2.5 concentration during the July 2017 was found to be 24.8μg/m3 which is below the EPA PM2.5 standard (35μg/m3). However, in many observations the PM2.5 concentration exceeded the EPA limit. The average PM10 concentration (26.4μg/m3) was far below the EPA standard (150μg/m3). PM1 was found to be the dominant size fraction during the summer measurements. The elevated PM2.5 concentration in such a rural area during summer could be due to the transport of the fine particles from more developed cities such as Astana to this region. This project is very much relevant to the Kazakhstan 2050 Strategy where environmental monitoring will be a requirement to protect public health. The outcome of this study will be critical to policy makers to plan for the future climate of Kazakhstan.

10MG.2

Trends in Particulate Matter Concentrations in Different Parts of Bangladesh. Munjurul Hannan Khan, MD. MASUD RANA, *Clean Air and Sustainable Environment Project*

Bangladesh suffers from severe air pollution, especially during dry season (November–April). Thick smog and dusts choke the country in this season every year. The country is densely populated, and a large number of rural and slum-dwelling people are exposed to such pollution. In this study, we investigated temporal and directional variations in PM concentrations in 8 district-cities located in different parts of the country. Hourly PM10 and PM2.5 concentrations in the middle (Dhaka, Gazipur, Narayanganj), south-east (Chittagong), north-east (Sylhet), south (Barisal, Khulna) and north-west (Rajshahi) of the country were captured using beta-attenuation method from 2013 to 2015. The data were quality controlled and analyzed with software “R” to understand seasonal, diurnal and directional characteristics of PM concentrations. Given importance to the capital city of Dhaka, long-range pollution to this city was also investigated - ninety-six-hour backward trajectories for the whole dry season were computed near the city using HYSPLIT model, associated with the corresponding PM concentrations and analyzed to trace long-range hotspots responsible for introducing pollutants into the atmosphere of Dhaka. The study found yearly PM10 concentrations in the stations about three times and yearly PM2.5 concentrations about six times greater than the national standards of Bangladesh. The country experienced several air pollution episodes in dry season when PM2.5 concentrations were 8–13 times greater than the World Health Organization (WHO) guideline value. Higher PM pollution and great contribution of fine particles most of the time were associated with the north-westerly wind. The city of Dhaka and its neighboring areas were found the most polluted among the cities. During winter (November to January) which was observed as the most polluted season, average PM10 concentrations in Dhaka, Gazipur, and Narayanganj were 257.1, 240.3, and 327.4 $\mu g\ m^{-3}$, respectively. Contributions of fine particles to the PM were also high in the winter season (>75%) compared to that in the wet season (~50%). Pollution levels during wet season (May–October) were, although found legitimate as per the national standards of Bangladesh, exceeded WHO guideline value in 50 % of the days. Trans-boundary source identifications using concentration weighted trajectory method revealed that the sources in the eastern Indian region bordering Bangladesh, north-eastern Indian region bordering Nepal and Nepal and its neighboring areas had high probability of contributing to the PM pollutions near Dhaka city.

10MG.3

Aerosol Chemistry at an Urban Site of Delhi: During Winter Fog Campaign. DEEWAN S. BISHT, Atul K. Srivastava, Sachin Ghude, Dilip Chate, P.D. Safai, P. Rao, R. Kulkarni, Suresh Tiwari, *Indian Institute of Tropical Meteorology*

During the foggy period (December 2015 to February 2016), the fine particulate matter (PM: diameter less than 2.5 micro meter) during the day and night time samples were collected at the Indira Gandhi International Airport New Delhi. The samples were weighted for mass concentrations and analyzed in the laboratory for chemical profiles of nine water-soluble inorganic ions (K+, NH4+, Na+, Ca2+,Mg2+, F−, Cl−, NO3- and SO42-), however, the carbon fractions (OC: organic carbon and EC: elemental carbon) is in progress. The concentrations of PM2.5 and its major chemical species were found large variability in their physical and chemical characteristics during the study period, which is due to the impact of meteorological conditions. The average concentration of PM2.5 was 230.9±185.9 µg m−3 which is 100 % of sampling days exceeding with the national ambient standard (40 µg m−3) and USEPA standard (12 µg m−3) which is seriousness for the regional atmosphere. The analysed chemical components in PM were 75.6 µg m−3 which is about 33% of the total mass concentrations. The concentration of total water-soluble inorganic species (PM2.5: 71.4 µg m-3and 79.7 µg m-3) during winter season was recorded higher day and nighttime respectively. A significant correlation was found between NH4+ and Cl−, SO42-, NO3- of PM2.5, which indicates the presence of ammonium salts (NH4Cl, (NH4)2SO4, NH4HSO4 and NH4NO3) and also indicates NH4+ as the major cation species for the neutralization of acidic components in the winter season. Whereas, in summer season Ca2+, Mg2+, Na+ and K+ were the alkaline species responsible for the neutralization of acidic components in the PM2.5 samples. In winter season the advection of air masses over the continental landmasses of Southern Afghanistan and Western region of Pakistan (winter season), and adjoining states of Delhi and could be the cause of higher PM2.5 aerosol over the studied region.

10MG.5

Comprehensive Analysis of Carbonaceous Gases and Particles in Beijing, 2016. SHUO YANG, Kebin He, Fengkui Duan, *Tsinghua University*

Carbon is one of the fundamental chemical elements and serves as the basic materials of all known life on earth. It could exist in gas or solid phase in the atmosphere, namely carbonaceous gases and particles. Carbonaceous particles (mainly refers to organic aerosol (OA) and elemental species) were the major components in $PM_{2.5,}$ which has caused extreme haze pollution around world, especially the North China Plain (NCP) region in recent decades, imposing detrimental effects on visibility, human health, and radiation forces.

Globally, around 20% of OA were primarily emitted (POA) and the rest were secondarily formed (that is, SOA, secondary organic aerosol). In urban site like Beijing, SOA could take up 30-77% of total OA concentration or even 44-71% of total PM2.5 mass, it was the crucial constituents of atmospheric particulates.

However, unlike other components in $PM_{2.5}$, detailed composition and chemical evolution of carbonaceous particle from gaseous precursors were intricate and poorly-analyzed. The integrated observation of carbonaceous gases and particles concentration and exploration of interior connections of gas-to-particle transformation is lacking.

In that case, we conducted a long-time continuous hourly-based observation and delineated the overall concentration level, diurnal variation profile of all carbon-species including carbon dioxide (CO_2), carbon monoxide (CO), methane (CH_4), volatile organic compounds (VOCs), non-methane hydrocarbon (NMHC), and particle organic carbon (OC), Elemental carbon (EC), water soluble organic compounds (WSOC) in Beijing, 2016.

The results indicated that unlike the inert carbonaceous gases (CO, CO_2 and CH_4) with one-peak in diurnal profile, the reactive VOCs/CO showed the double-peak pattern, with a pronounced peak at midnight, the same as carbonaceous particle OC/EC ratio and $WSOC_1/WSOC_{2.5}$ (WSOC in PM_1 and $PM_{2.5}$, respectively) ratio, especially in winter.

high positive relationship between carbonaceous particles with VOCs precursors level (OC-VOCs, $WSOC_1$-VOCs, $WSOC_{2.5}$-VOCS), and meteorological RH condition (RH-OC and RH-WSOC) were observed (with R-sqaures above 0.75), indicating VOCs and RH were the major factors facilitating high organic mass accumulation in the atmosphere. Moreover, RH with different ranges imposed different influence on WSOC concentration in PM_1 and $PM_{2.5,}$ respectively. $WSOC_1$ concentrations were enhanced largely with RH ranging from 50% -80%, but for $WSOC_{1-2.5}$ formation, the corresponding RH level changed to larger than 80%.

An F-factor method (based on logarithmic calculation of carbonaceous particles concentration (μgC m^{-3}) divided by that of carbonaceous gases) was established to reflect gas-particle relationship of carbon and has been verified effective in indicating the haze events and revealing the existence form of carbon in the atmosphere. higher F-factor in winter indicated that carbon was prone to exist in particle phase in Beijing. And higher F-factor (>0.15) corresponded with $PM_{2.5}$ load larger than 150 μg m^{-3}, while a lower value (<0.05) reflected a clean condition ($PM_{2.5}$ less than 35 μg m^{-3})

In this work, we provided the first comprehensive mass closure observation of all carbonaceous gases and particles in the atmosphere, which helped broaden our understanding in carbon cycle and secondary organic aerosol formation. Our new insights into SOC formation may contribute to an accurate evaluation of conversion from carbonaceous gases to particles, specifically, the effect on WSOC formation from VOCs precursors in the atmosphere.

10MG.6

Source Apportionment of Absorbing Aerosols (Soot Particles) in Delhi, India during a Highly Polluted Period (Wintertime). SURESH TIWARI, Rajan K. Chakrabarty, Umesh C. Dumka, Atul K. Srivastava, Deewan S. Bisht, Philip K. Hopke, *Indian Institute of Tropical Meteorology*

Urban areas in the developing countries are major sources of carbonaceous aerosols requiring detailed assessment of the concentrations and source apportionment in order to attain improved air quality. A seven-wavelength Aethalometer (Magee Scientific model AE-33) was utilized to measure the spectral absorption coefficient (babs) at 7 wavelengths and estimate Black Carbon (BC) mass concentrations in Delhi during a winter research campaign (December 2015 – February 2016). The Aethalometer measurements were supported by measurements of PM10 and PM2.5 concentrations and air-pollution gases (NOx, CO, and O3) as well as by Photoacoustic Extinctiometer (PAX) measurements of scattering, absorption coefficients, and single scattering albedo (SSA). From the measured babs, the Angstrom Aerosol Exponents (AAE) was estimated at 370, 470, 880, and 950 nm. Assuming values of AAE=1.0 and AAE=1.8 for the fossil-fuel combustion and biomass burning particles, respectively, the BC components (BCff and BCbb) were estimated via the "Aethalometer model". Very high PM10 (246 ± 110 µg m-3) and PM2.5 (146 ± 70 µg m-3) concentrations were measured during the campaign period. BC represented a large fraction of the PM mass (9.8% to PM10 and 16.5% to PM2.5). The BC concentrations varied from 3.2 to 59.9 µg m-3 (mean of 24 ± 12 µg m-3) depending strongly on meteorological conditions i.e., changes in mixing layer height and dispersion, and on the differences in carbonaceous emission rates. The highest BC concentrations were observed during the nighttime and early morning hours. Fossil-fuel BC (BCff) was emitted by traffic, industrial sources, and domestic use of natural gas. Combustion of wood, waste material, dung cakes, and agricultural crop residue burning produced the BCbb. The highest contributions of BCff to BC were found during late-night hours and in the early morning (~03:00-08:00 hrs Local Standard Time: LST). On some days, high BCff was found until noon (~13:00 hrs LST). Large contributions of the BCbb to total BC were found during the early evening-to-night hours (~18:00 – 24:00 hrs LST) likely from increased domestic biofuel burning for cooking and heating as well as open fires in the roads during the cold winter nights. BCff and BCbb were strongly related to CO and NO emissions indicating common local primary combustion emissions. In general, higher BCff/BCbb values were associated with lower SSA values. A sensitivity analysis was performed to assess the BC source apportionment (i.e., BCff/BC and BCbb/BC) by changing the wavelength pairs and the AAEff and AAEbb values. The results showed that the "Aethalometer model" was more sensitive to changes in AAEff compared to AAEbb values. Although both sources of BC are important, biomass burning continues to deteriorate local air quality within and around urban environments in India and necessitates appropriate measures to mitigate the effects of BC on climate, ecosystems, and human health.

10MG.8

Air Quality Status in India: Chemical Characterization and Source Interpretation of a Few Major Cities. RANJIT KUMAR, *DEI, Dayalbagh, Agra*

Air quality of any airshed can be adjured by aerosol particles. Recently, WHO has reported that out of the 20 most polluted cities in the world 13 are from India. This is worrisome. The concentration of the respirable suspended particulate matter (PM10) and fine particulate matter (PM2.5) are high for most of the cities in India except Tirupati. The concentrations of PM10 and PM2.5 over megacities like Agra, New Delhi, Chennai, Kanpur, Pune, Mumbai, Kolkata are quite higher than WHO, USEPA, EUPAQ standards even the concentration are many times higher than National Ambient Air Quality Standard (NAAQS) set by India. Aerosol particle causes radiative forcing affects climate and pose threat to human health. The effects of aerosol particles depend upon the chemical constituents of aerosol. A long-term study on chemical characterization of aerosol particle has been carried out in Agra over the Indo-Gangetic basin. The concentration of NH4+ is highest followed by Mg2+>Ca2+ >SO42->Cl->K+>NO3->Na+. The sum of cations is higher than the sum of the major anions. The aerosol is alkaline in nature over this region. The ratio of SO42- and NO3- upon Ca2+, Mg2+, NH4+, Cl- is less than 1. The NH4+, Ca2+, Mg2+, are a main neutralizing component of the aerosol over this region. Principle component analysis (PCA) reveals soil as a major contributor of aerosol particles over this region. Increase in the number of vehicles and construction activities are other important sources. Biomass combustion and open waste burning also contribute towards high concentration of the aerosol particle in this region. A comparative study on chemical constituents of aerosol particles of New Delhi, Kanpur, Pune, Mumbai, Kolkata has been performed. The concentration of chemical constituents of aerosol particulate is different in different cities but the trends are more or less similar. The natures of the aerosol of all these megacities are basic. But the source strength is different at different places. The concentration of aerosol particle Hysplit model and wind rose studies have shown the role of meteorological parameters and condition in the concentration of aerosol particle over the mega cities of India.

10MG.9

New Particle Formation and Severe Haze Events in Beijing, China. ROHAN JAYARATNE, Buddhi Pushpawela, Lidia Morawska, Hui Li, Jian Gao, *Queensland University of Technology, Brisbane, Australia*

An estimated 2.5 million people in China die each year from the health effects of indoor and outdoor air pollution. The concentration of airborne pollutants in China's megacities can reach many hundreds of times that of European and American cities. Severe haze pollution events are routinely observed in Beijing over the winter months, with $PM_{2.5}$ levels often exceeding 10 times the China National Ambient Air Quality Standard. The formation and evolution mechanisms of these haze events are not fully understood. In addition to the nature of the emission sources, it is known that there is a significant influence of meteorological conditions such as wind direction and speed, temperature and humidity. Some studies have shown that the haze particle concentrations are driven to a large extent by secondary aerosol formation.

We carried out a detailed study of the pollution in Beijing over three consecutive months from November 2015 to January 2016 using a suite of instrumentation to monitor particle number and mass concentration and a range of gaseous concentrations. Explosive haze events were observed on five occasions where the $PM_{2.5}$ concentration increased ten-fold within a few hours and lasted at these high values for up to 2-3 days. The corresponding increase in particle number concentration was less than two-fold. Particle number size distributions were measured using a scanning mobility particle sizer (SMPS) and new particle formation (NPF) events were monitored with a neutral cluster and air ion spectrometer (NAIS). The SMPS and NAIS monitored particles in the size ranges 10-400 nm and 2-42 nm, respectively. The combination of these two instruments enabled a clear differentiation between NPF events and growth events. NPF events were observed only during the periods between the haze events when the winds arrived from the cleaner areas to the north of the city. The results suggest that weak southerly surface winds and high humidity were responsible for the severe haze pollution events, rather than an abrupt increase in emissions. Deeper temperature inversions and lower boundary layers contributed to stronger accumulation of pollution in the city.

There was some evidence that the secondary particles formed during NPF events contributed to the subsequent haze events, but the meteorological data suggests that the majority of the particles originated within the city, with a less significant contribution from the industrialized south and east. Investigation of the chemical composition of the particles revealed a significant increase in sulphates, nitrates, ammonium and potassium during the haze events, with only a marginal increase in chlorides, magnesium and calcium. Concentrations of oxides of nitrogen and carbon monoxide also showed a sharp increase at these times suggesting that the haze originated from combustion sources.

The NAIS also provided information on the charge carried by particles in the air. On a normal day, approximately 15% of particles were charged. During an NPF event, this fraction decreased to about 10%. In contrast, during haze episodes, it increased to between 20% and 30%. This is explicable in terms of the mean particle size; haze particles are much larger than secondary particles. It is known that the fraction of particles that are charged increases sharply with size. It should be noted that the reported fractions refer to particles that are smaller than 42 nm – the upper size cut-off of the NAIS. During haze events, as confirmed by the SMPS, a large proportion of the particles are larger than this size. The proportion of particles that are charged increases sharply with size and, therefore, it is to be expected that the actual fraction of all particles that are charged during a haze episode is much larger than 30%.

10MG.12

Concentrations and Fluxes of Black Carbon in Beijing Using Single Particle Soot Photometry Measurements.

RUTAMBHARA JOSHI, Dantong Liu, James Allan, Hugh Coe, Michael Flynn, Ben Langford, Eiko Nemitz, Neil Mullinger, Freya Squires, Adam Vaughan, James Lee, Yele Sun, Pingqing Fu, Simone Kotthaus, *University of Manchester*

Black carbon (BC) forms an important component of particulate matter globally, due to its impact on the climate, environment and human health. Megacities such as Beijing are hotspots of BC emissions and due to rapid urbanisation and development their sources are uncertain and rapidly changing. Therefore, identifying and quantifying these emission sources is critical for effective policy making and achieving the desired reduction in air pollution. In this study, at an urban location in Beijing, we present the first ever direct measurements of BC fluxes using eddy correlation. The measurements were made as part of a large joint UK-China field experiment, during winter 2016 (November-December) and summer 2017 (May-June). We focus on characterising BC properties, particularly its mixing state, through analysis of the size and coating content of individual particles. This allows us to attribute individual particles to potential sources. We then use eddy correlation to separately calculate BC fluxes for each of the different sources. The Single Particle Soot Photometer (SP2) was used to uniquely quantify the morphology independent mass of single refractory BC particles and their coating content. Black carbon was measured at 5 Hz from an inlet placed at 102 m height, adjacent to a 3D sonic anemometer. From the covariance between concentrations and vertical wind speed emission fluxes can be calculated over flux footprints of several square kilometres, using the eddy covariance method. In this paper, BC characterisation and flux analysis will be presented for both winter and summer seasons using four weeks of continuous data, which includes several severe haze pollution events. The analysis identified distinct modes for sizes and coating thickness of BC containing particles in summer and winter, which indicates a variation in their source origin (traffic, coal and biomass burning). The fluxes will provide further insight into the complex environment of Beijing, allowing us to identify and quantify contributions of local emission sources.

10MG.13

Exposure Profiles and Related Health Risks of Benzene Toluene and Xylene at Two Different Microenvironments of a Terai Region in North India. AMIT MASIH, *St. Andrew's College, Gorakhpur, India*

Benzene, toluene and xylene (BTX) are elements of an important group of aromatic volatile organic compounds (VOCs) that are usually emitted from various sources. BTX play a vital role in the tropospheric chemistry as well as pose health hazard to human being. Thus, an investigation of ambient benzene, toluene and xylene (BTX) was conducted at an urban and rural site in Gorakhpur for a span of one year in order to ascertain the contamination levels. Sampling and analysis of BTX were performed using a methodology based on NIOSH method 1501. BTX were sampled by drawing air through activated coconut shell charcoal tubes, using a low-flow SKC Model 220 sampling pump at the flow rate of 250 ml/min for 20-24 hrs. The air suction rate was verified every week using calibrated rotameters with an accuracy of ±1%. The samples were extracted with carbon disulphide by occasional agitation and the aromatic fraction was subjected to GC-FID. Total mean concentration of BTX was 30.95 µg/m3 in all the samples and the total range was from 3.4 µg/m3 to 45.4 µg/m3 with the median of 24.8 µg/m3. The maximum levels of total BTX was found to be 39.3 µg/m3 in winters, followed by 28.4 µg/m3 in summer and 25.1 µg/m3 in monsoon season. The total BTX concentration was highest at rural site (11.8 µg/m3) followed by urban site (8.8 µg/m3). At both the sites, maximum B/T ratio was found in winter season whereas the X/B ratio was found to be lowest. Toluene against benzene plot shows R2 value of 0.91 and 0.93 at urban and rural sites respectively. At both the sites, the estimated integrated lifetime cancer risk (ILTCR) for benzene exceeded the threshold value of 1E-06 whereas the individual hazard quotients (HQ) for BTX did not exceed unity at any of the sites.

Keywords: Ambient BTX, Urban & rural microenvironments, Terai zone, Health Risks

10MG.14

Formation and Characteristics of Secondary Aerosols in an Industrialized Environment during Cold Seasons. Yangzhou Wu, XINLEI GE, Junfeng Wang, Mindong Chen, *Nanjing University of Information Science and Technology*

Secondary aerosols including inorganic and organic components often dominate the fine aerosol mass, it is thus important to elucidate the formation and characteristics of these species. In this work, we measured the submicron aerosols (PM1) by using an Aerodyne high resolution soot-particle aerosol mass spectrometer in suburban Nanjing, China. The site was surrounded by industry plants, and the measurement was conducted during cold seasons (February-March 2015). We found that under such environment, the PM1 was predominantly comprised of secondary species (on average 63.2% from ammonium sulfate and nitrate). Results show that moisture plays a key role to enhance both nitrate and sulfate formations. The moisture promotes the gas-particle partitioning and nocturnal heterogeneous production of nitrate, while transformation of SO2 into sulfate directly in aqueous phase is more significant. The organic aerosol (OA) occupied ~1/4 of total PM1 mass, and the primary OA (POA) and secondary OA (SOA) contributions were almost equal. A specific industry-related OA was separated and a modified graphical method was introduced to describe the evolution of OA. Results further show that the most abundant OA factor, which is the one with highest oxidation degree, is also mainly driven by aqueous-phase processing, while the other two less oxygenated SOA factors are mainly governed by photochemical processing. Peak sizes of sulfate, nitrate and OA all shifted towards larger sizes with the increases of relative humidity, reflecting the effects of aqueous-phase processing too. Aqueous-phase driven secondary aerosols were found to be very important in enhancing the PM1 pollution, while photochemical processed SOA was important to OA pollution, leading to a fresher OA at higher OA concentrations. We further demonstrated influences of the aqueous-phase processing and photochemical processing on formation of secondary aerosols by using two typical cases, respectively. This paper highlights the importance of aqueous-phase chemistry on sulfate and nitrate formations, and that different portions of SOA can be dominated by different mechanisms in an industrialized environment.

10MG.15

Study of Influence of Rain on Ambient PM in Indian Cities. SWETHA PENDYALA, Sreekanth Bojjagani, Rakesh Kumar, Virendra Sethi, *IIT Bombay*

The Central Pollution Control Board has listed 94 cities that are non-compliant for PM10 as per National Ambient Air Quality Standards. An effort is underway to develop action plans for mitigation of ambient air particulate matter in ten such cities in Maharashtra. Ambient air quality is monitored under the National Ambient Air Monitoring Program (NAMP) and the State Ambient Air Monitoring Program (SAMP). An analysis of historical data was carried out using the NAMP and SAMP datasets for the cities of Amravati, Aurangabad, Chandrapur, Kolhapur, Mumbai, Nagpur, Nashik, Navi Mumbai, Pune and Solapur. In some of these cities, road dust was found to be a major contributor to the ambient PM. An initial analysis of seasonal data indicated that such dust is suppressed by rainfall. The same was also verified using data from Continuous Ambient Air Quality Monitoring Stations from Nashik and Pune for episodic rains, and additionally for Chandrapur also by using real time measurements at eleven locations. Particle size distribution measurements were carried out using MOUDI in Chandrapur on a dry day and a subsequent day when it had rained. The results showed a bimodal distribution on the dry day, while on the day with rain, the larger size mode was suppressed. The results provide insights into the extent of contribution from fugitive dust sources, and are currently being used to develop control strategies.

10MG.16

Variations of PM2.5 Chemical Components and Its Source Apportionment during Winter Season from 2013 to 2017 in Beijing of China. HEZHONG TIAN, Panyang Shao, Huanjia Liu, Bobo Wu, Weizhao Liang, Shuhan Liu, *School of Environment, Beijing Normal University*

By analyzing the chemical components (water-soluble inorganic ions, carbonaceous components and trace elements) of multi-size airborne particles (PM2.5, PM1, PM10) sampled from December 15, 2016 to January 15, 2017 in Beijing, as well as the associated gaseous pollutants and meteorological parameters, we investigated the variation characteristics between haze and normal days and compared them with the well-documented haze episode in January 2013. Higher ambient temperature (AT), higher relative humidity (RH) and low wind speed (WS) are common meteorological characteristics during winter haze periods. With strict atmospheric pollution control measures over the past four years, concentrations of SO2, SO42- and most anthropogenic elements have decreased whereas NO3- and NH4+ concentration in PM2.5 increased by as high as 77.9% and 47.3% respectively in the sampling period of 2016-2017 winter compared with January 2013. Secondary inorganic aerosol (SIA) increased sharply and significantly aggravated haze episodes, in which nitrate has replaced sulfate to be the dominating component in PM2.5 although the rapid growth of sulfate still played an important role in the formation and evolution of extremely heavy haze events. With ammonium-rich condition and high RH, NO3- was thought to mainly be produced by enhanced heterogeneous reactions. The heaviest Cross 2017 New Year's Haze episode was characterized by strong secondary reactions and external transport of anthropogenic pollutions from south of Beijing. In consequence, it can be concluded that urban air pollution in Beijing has shifted from being dominated by coal burning to a mix of vehicle emissions and coal burning. It's quite crucial to cut NOx, NH3 and SO2 emissions simultaneously and strengthen inter-regional air pollution prevention and control work in preventing winter haze in Beijing.

10MG.17

Winter Time Aerosol Size Distribution Study Across Three Sites in Delhi. Suneeti Mishra, S.N. TRIPATHI, Deepika Bhattu, Varun Kumar, Suresh Tiwari, Atul K. Srivastava, Deewan S. Bisht, *IIT Kanpur*

Particle size distribution, mass and number were measured at three sites in Delhi, during the winter of 2017.These sites were at different locations with distinct land–use patterns and sources contributing to air pollution. Vehicular emissions being the dominant source at all the three locations. Particle size distribution helps us to better understand about the sources and various atmospheric processing like aging. At all the three sites, a set of Scanning Mobility Particle Sizer (SMPS) and Optical Particle Sizer (OPS) were deployed which collectively measure size selected aerosols from ultrafine (13 nm) to coarse (10 µm) range. At the third site an additional Aerodynamic Particle Sizer (APS) measured from 0.5 µm up to 20 µm was also deployed giving a deeper insight into the coarse range. Individual distributions were merged to give wide range size distributions and understanding the mode formation at all the sites. Their temporal and spatial variation along with the diurnal properties was closely studied to understand the particle formation and the time of the day to find their source. The distributions were of three types unimodal, bimodal and trimodal depending on the time of the day. During the afternoon and evening session modes increased in the nucleation and accumulation range as compared to morning. Strong nucleation and accumulation modes observed at all three sites at different time interval suggest the different sources responsible for the particulate matter.

10MG.18

Ambient Particle Formation and Growth in Mexico City. LUCIA CAUDILLO, Dara Salcedo, Oscar Peralta, Telma Castro, *National University of Mexico*

Studies of the size distribution of fine particles in Mexico City are very scarce. Baumgardner et al. (2000) reported the size distribution of particles between 100 and 700 nm during two weeks in November 1997, in a Natural Reserve south of Mexico City. The variability observed in the concentration of the Aitken and accumulation modes was related to concentrations of CO and O3, suggesting a link between the emission of primary aerosols and condensational growth. Dunn et al. (2004) measured the size distribution of nanoparticles between 3 and 48 nm and observed several nucleation events related with high SO2 concentrations during the morning, and low PM10 and PM2.5 concentrations in the afternoon. However, there has not been any other report of particle size distributions in Mexico for 13 years.

In this work, we will describe measurement of size distributions of particles between 10 and 400nm in Mexico City, using a TSI Scanning Mobility Particle Sizer Spectrometer (SMPS), during 30 days from October to November, 2016. Three different cases were observed during this period. The first one corresponds to new particle formation during high SO2 events. The second one, probably due to secondary formation processes, occurs at midday and is related to high solar radiation and ozone concentrations. The third one is related to the emission of primary nanoparticles from combustion sources.

10MG.20

Composition and Characteristics of NR-PM1 Using HR-TOF-AMS over a Big Urban City of Western India. ATINDERPAL SINGH, Rangu Venkata Satish, Neeraj Rastogi, *Physical Research Laboratory, Ahmedabad, India*

Poor understanding on the characteristics and composition of non-refractory PM_1 (mainly secondary aerosol) leads to large uncertainty in the assessment of their effects on air quality and climate. Towards this, it is important to study and understand their composition, characteristics and temporal evolution in different regions. Present study reports real-time characteristics of non-refractory submicron aerosol ($NR\text{-}PM_1$) using high-resolution time-of-flight aerosol mass spectrometer (HR-ToF-AMS) during post-monsoon season over a big urban city (Ahmedabad, 23.0 ^{o}N, 72.6 ^{o}E, 49m amsl) situated in a semi-arid region of western India.

Study region receives most of annual rainfall during monsoon season (June-September), which cleans up the atmosphere. Subsequently, primary and secondary aerosol start accumulating in the atmosphere. During a month-long study (September 19th to October 19th, 2017) started right after monsoon season, $NR\text{-}PM_1$ varied from 1.9 to 102 µg m^{-3} (14±9.8 µg m^{-3}; Avg±1σ), where $NR\text{-}PM_1$ is composed of organic aerosol (OA), SO_4^{2-}, NO_3^-, NH_4^+ and Cl^-. All the species of $NR\text{-}PM_1$ showed increasing trends in their mass concentrations with higher slope for OA. These changes in concentrations of species reflect the role of local/regional sources and atmospheric processes in charging up the atmosphere. OA was observed to be dominant contributor to $NR\text{-}PM_1$ with the contribution of 55%, followed by sulfate (31%), and contribution of other ionic species were ≤ 11%. Aerosol neutralization ratio (ANR, defined as the molar ratio of NH_4^+ to sum of SO_4^{2-}, NO_3^- and Cl^-), an indicative of aerosol acidity, has a period average value of 0.85±0.07 with the highest value during afternoon hours (~0.91).

Diurnal trends exhibited lower O/C and higher H/C ratios during rush hours (peak at 08:00 and 20:00 hrs IST), which indicates the dominance of primary organics from vehicular emissions at these hours. Strong photochemical activity during afternoon hours was evident from high O/C ratios that leads to enhancement in organic mass due to secondary formation during these hours. Moderate peak in O/C at 04:00 hrs could be due to oxidation of precursors by nocturnal oxidants. Slope of Van Krevelen (O/C vs H/C) diagram is often used to understand the bulk composition of OA. In this study, it is found to be -0.77±0.35, which suggests that ambient OA is aging towards widely observed slope (-1) of OA i.e., carboxylation. It also infers that the observed OA was a variable mixture of fresh and aged OA during the study period. This study provides deeper insights of secondary aerosol abundances in ambient air, hither to lacking from this region.

10MG.21

Investigating the PM2.5 and PM10 Concentrations over the Atmosphere of Iran and Its Major Cities Using Satellite Observations. Zhuldyz Darynova, Hamed Sharifi, Soudabeh Gorjinezhad, MEHDI AMOUEI TORKMAHALLEH, *Chemical and Aerosol Research Team, Nazarbayev University*

Particulate Matter (PM) is one of the most important air quality concerns in Iran where has been recently experiencing critical dust issues transported from neighbor countries around the Persian Gulf including Kuwait and Saudi Arabia, and generated locally. For example, the PM2.5 and PM10 concentration in the city of Ahwaz were reported to reach the maximum values of 910 (69 in average) and 5337 (319 in average) µg/m3 from April to September 2010. Although the ground based measurement is referred to as accurate method, due to limited area coverage, irregular distribution of stations and expensive instruments, researchers are seeking alternative methods. Particularly, such instruments needs to be upgraded and calibrated in Iran. In our study we develop several statistical models to utilize satellite based measurements and evaluate capability of method in predicting PM10 and PM2.5 concentrations over the atmosphere of Iran. Specifically, the Moderate Resolution Imaging Spectrodiometer (MODIS), instrument on board of the satellite Terra and Aqua from the NASA allows us to estimate ground-level PM10 and PM2.5. It is achieved by determining Aerosol Optical Depth (AOD) which reflects optical characteristics of aerosols. The current study is focused on estimating PM10 and PM2.5 over six cities of Iran: Tehran (heavy traffic), Ahvaz (transported dust), Ghaemshahr (relatively clean), Isfahan (industrially polluted), Mashhad (developing city) and Tabriz (cold climate) from 2012 to 2017. The findings of this study will demonstrate the strong potential of satellite remote sensing, which may provide a cost-effective approach as a source of information for estimation of ground-level particle concentrations. Furthermore, it provides key information for policy makers to adapt new regulations and infrastructure to improve the air quality in major cities of Iran.

10RA.1

Aerosol Optical Absorption Properties at a High Mountain Site in the Western Mediterranean. Jose Nicolás, Nuria Galindo, Ramón Castañer, Eduardo Yubero, Javier Crespo, Carlos Pastor, FRANCO LUCARELLI, Giulia Calzolai, Silvia Nava, *Miguel Hernández University, Elche, Spain*

Measurements of particulate matter (PM), absorption coefficient (σ_{ap}) and Absorption Angstrom Exponent (AAE) have been performed during three years (2014-2016) at a remote site (1558 m a.s.l) located in the southeast of the Iberian Peninsula, close to the Mediterranean coast. Mean values ± (standard deviation) of the measured parameters were: PM_{10} (11.3±19.8 $\mu g\ m^{-3}$), σap (2.18±1.45 Mm^{-1} / λ=520 nm) and AAE (1.190±0.225). PM concentrations and σap were maxima during summer, while AAE values were highest during the colder months, as expected for high altitude environments with scarce human activity. The influence that both, air masses coming from the Sahara desert loaded with mineral dust (SDE) and the height of the Planetary Boundary Layer (PBL), had on the studied parameters was also analyzed. During SDEs, σ_{ap} and AAE levels increased. These increments were slightly higher when the sampling point was located within the free troposphere (FT) and correlated with the intensity of the event. In the case of SDEs with high mineral dust (MD) concentrations, AAE values increased up to 30% and σap values were more than double compared to average values for non-event days. However, the seasonal variability of the optical parameters could not be attributed to these episodes since the MD load at the sampling point did not show significant seasonal differences. For this reason, the different spectral absorption behavior observed between the warmest and the coldest months may be attributed to the seasonal differences in the percentage contribution of Brown Carbon (BrC) to PM levels. These results indicate that for short wavelengths (UV and VIS), the absorption due to non-BC absorbers during the winter was almost twice that registered during summer time.

10RA.2

Sources for Atmospheric Aerosol at Oliktok Point, Alaska. JANEK UIN, Gunnar Senum, Stephen Springston, *Brookhaven National Laboratory*

Oliktok Point in Alaska is the new site for the U.S. Department of Energy Aerosol Observing System (AOS) AMF 3, which was deployed there in August 2016 as part of the DOE Atmospheric Radiation Measurement (ARM) project. The site is located close to the shore of the Arctic Ocean and is surrounded by tundra with several oil processing plants nearby. The station has complement of instruments for measuring trace gas concentrations, aerosol particle number concentrations, particle size distributions down to 60 nm, and particle optical and hygroscopic properties.

Measurement data suggests that the atmospheric aerosol at Oliktok Point is a mixture from a few distinct local and remote sources with the aerosol properties having a strong correlation with the wind direction.

Winds from the north, from the direction of the ocean shore, usually bring clean air masses with very low particle counts and a particle hygroscopic growth factor at around 1.5, which is common for sea spray. However, occasionally higher particle counts can be observed, most likely originating from the main building of the Oliktok Long Range Radar Site, located close by almost due north from the measurement site.

The prevalent wind direction at the site is from the east and is associated with elevated particle counts and larger mean particle sizes. The largest oil processing plant in the region is located in Prudhoe Bay, which is 60 km east from the site and is the most likely candidate for these emissions.

As the power generators for the site are located close by to the south of the AMF 3 measurement container, the southerly winds bring diesel emission plumes characterized by very high particle counts, elevated CO concentrations and high light absorption.

10RA.3

Airborne Atmospheric Aerosol Measurement System. YONG-HEE PARK, Kang-Ho Ahn, *Hanyang University, R. of Korea*

It is important to understand the atmospheric aerosols compositions and size distributions since they greatly affect the environment and human health. Particles in the convection layer have been a great concern in global climate changes. To understand these characteristics satellite, aircraft, and radio sonde measurement methods have usually been used. An aircraft aerosol sampling using a filter and/or impactor was the method commonly used (Jay, 2003). However, the flight speed particle sampling had some technical limitations (Hermann, 2001). Moreover, the flight legal limit, altitude, prohibited airspace, flight time, and cost was another demerit. To overcome some of these restrictions, Tethered Balloon Package System (T.B.P.S.) and Recoverable Sonde System(R.S.S.) were developed with a very light optical particle counter (OPC), impactor, and condensation particle counter (CPC). Not only does it collect and measure atmospheric aerosols depending on altitudes, but it also monitors the atmospheric conditions, temperature, humidity, wind velocity, pressure, GPS data, during the measurement (Eun, 2013). In this research, atmospheric aerosol measurement using T.B.P.S. in Ansan area is performed and the measurement results will be presented. The system can also be mounted to an unmanned aerial vehicle (UAV) and create an aerial particle concentration map. Finally, we will present measurement data using Tethered Balloon Package System (T.B.P.S.) and R.S.S (Recoverable Sonde System).

10RA.5

Comparison of Desert Aerosol Optical Characteristics of Ouarzazate (Morocco) and Sevilleta (New Mexico).

Abdelouahid Tahiri, MOHAMMED DIOURI, Jamal Barkani, *Atmospheric Physic, LME, University of Oujda, Morocco*

Sun-photometer columnar measurements of 2017, at Sevilleta (34.35N, 106.88W) and Ouarzazate (30.92°N, 6.91°W) AERONET sites allowed the determination of microphysical and optical characteristics of such different desert aerosol where both Saharan mineral dust (for Ouarzazate) and clear sky weather are observed depending to the season. The aerosol optical depth at 0,5 µm show high values with annual means of 0.30 ± 0.15 at Ouarzazate close to the Sahara and 0.08±0.03 at Sevilleta. The single scattering albedo monthly averages range from 0.45 to 0.90 with almost the same values for six months. The shape of the volume distributions of the particles are very different with very high amplitudes at Ouarzazate mostly for coarse mode (0.127±0.096 µm3/µm2), and with significant deviations of the respective median radii. All the results confirm the character of each site.

Despite the great differences in microphysical characteristics, the aerosol radiative forcing efficiency (month means) for visible wave seems having the same seasonal variation at bottom and at Top of the atmosphere. Near the Sahara or in the American continental desert, aerosols seem to act with the same tendency of radiative forcing, the surface albedo having a very important moderating role.

10RA.6

Short-interval Aerosol Water-soluble Inorganic Ions Observed under the Influence of Upslope Wind, Transported Biosmoke, and Fog at Mountain Lulin, Taiwan. CHUNG-TE LEE, Wei-Ren Chen, Shih-Yu Chang, Charles C.K. Chou, Neng-Huei Lin, *National Central University, Taiwan*

Field campaigns were conducted at Lulin Atmospheric Background Station (LABS) from October to November 2015 and March to April 2016. Short-interval variations of water-soluble inorganic ions (WSIIs) of $PM_{2.5}$ (an aerodynamic diameter equal to or less than 2.5 µm) were monitored using particle-into-liquid sampler coupling with ion chromatographers (PILS-IC). Meanwhile, $PM_{2.5}$ mass concentration, PM_{10} and PM_1 aerosol absorption and scattering coefficients, aerosol total number concentration, aerosol number and volume size distributions, and gaseous pollutants were also measured at LABS.

The comparisons of WSIIs (SO_4^{2-}, NO_3^-, NH_4^+, and K^+) between integrated PILS-IC data and collocated filter samples indicated that the measurements were consistent ($R^2 \geq 0.75$) with each other. In autumn sampling, upslope wind resulted in an increase of $PM_{2.5}$ from 6.9 ± 2.1 to 11.5 ± 2.3 µg m^{-3} in average. During the spring campaign, five-day backward trajectories were mostly originated from far west of Indochina in March but changed to from the Philippines in April. The average $PM_{2.5}$ mass concentration of spring (17.5 ± 7.89 µg m^{-3}) was more than twice that of autumn (8.0 ± 2.9 µg m^{-3}) after excluding rainy periods. Transported biomass burning (BB) smoke form Indochina was verified to cause high $PM_{2.5}$ mass concentration in spring, which, however, masked upslope wind effects. Ion equivalent evaluation indicated that the molar ratio of $[NO_3^-]/[SO_4^{2-}]$ increased linearly as the molar ratio of $[NH_4^+]/[SO_4^{2-}]$ exceeded beyond 1.5. During the BB period, the molar ratio of $[NH_4^+]/(2[SO_4^{2-}]+[NO_3^-])$ at 0.88 ± 0.25 showed a near complete neutralization among major ions in spring. In the third to fifth selected BB events, average $PM_{2.5}$ mass concentration was 24.9 ± 12.7 µg m^{-3}, while average NH_4^+, SO_4^{2-}, NO_3^-, and K^+ concentration were 1.7 ± 1.0, 3.7 ± 1.4, 1.4 ± 1.0, and 0.3 ± 0.2 µg m^{-3}, respectively. Excess NH_4^+ (after neutralizing with SO_4^{2-}) correlated well with NO_3^- ($R^2 \geq 0.70$) indicating NO_3^- was formed through homogenous gas phase reactions. Four fog events occurred in the three selected BB events, aerosols were observed either diluted by clean air or grown in fog. In addition, aerosol number size distributions presented a unimodal distribution during BB events, while bimodal distributions were observed in the fog events.

10RA.7

Organic Nitrogen in Aerosols at a Forest Site in Southern Appalachia. XI CHEN, Mingjie Xie, Michael Hays, Eric Edgerton, Donna Schwede, John Walker, *US Environmental Protection Agency*

This study investigates the composition of organic particulate matter ($PM_{2.5}$) in a remote montane forest in the southeastern U.S., focusing on the role of organic nitrogen (N) in sulfur-containing secondary organic aerosol (SOA) and in biomass burning aerosols .The average fraction of water soluble organic nitrogen (WSON) in water soluble total nitrogen (WSTN) exhibited a pronounced seasonal pattern, ranging from ~18% w/w in the spring to ~10% w/w in the fall. Nitro-aromatic and nitrooxy-organosulfate compounds accounted for as much as 28% w/w of WSON. Oxidized organic nitrogen species showed a maximum concentration in summer (average of 0.65ngN/m^3, maximum of 1.83ngN/m^3) consistent with greater relative abundance of aged biogenic SOA tracers (higher generation oxygenated terpenoic acids). Highest concentrations of nitro-aromatics (e.g., nitrocatechol and methyl-nitrocatechol) were observed during the fall season impacted by aged biomass burning plumes. Isoprene derived organosulfate (MW216, 2-methyltetrol derived), which is formed from isoprene epoxydiols (IEPOX) under low NOx conditions, was the most abundant individual organosulfate. Although nitro-aromatics and nitrooxy organosulfates account for a small fraction (seasonal averages of 1.0 to 4.4%) of WSON, our results provide insight into atmospheric formation processes and sources of these largely uncharacterized organic nitrogen species.

10RA.8

Simulation of Marine Aerosols over the East China Sea Using WRF/CMAQ Modeling System. Mingjie Kang, PENGFEI WANG, Pingqing Fu, Hongliang Zhang, *Louisiana State University*

Marine aerosols exert a strong influence on global climate change and biogeochemical cycling, as oceans cover beyond 70% of the Earth's surface. However, investigations on marine aerosols are relatively limited at present due to the difficulty and inconvenience in sampling marine aerosols as well as their diverse sources. East China Sea (ECS), lying over the broad shelf of the western North Pacific, is adjacent to the Asian mainland, where continental-scale air pollution could impose a heavy load on the marine atmosphere through long-range atmospheric transport. In this study, two-month (May and June in 2014) marine air quality simulation using Weather Research and Forecasting (WRF) model and the Community Multiscale Air Quality (CMAQ) model was conducted to understand PM2.5 and its chemical components over ECS. Multi-resolution Emission Inventory for China (MEIC) was used for anthropogenic emissions and model performance was validated by comparing observation data obtained over the ECS and coastal cities. The model simulations indicate a significant influence of terrestrial outflow of continental aerosols on the marine atmosphere, which is particularly obvious in days with high abundance. This study demonstrates that CMAQ model can reproduce spatial distribution and concentration of marine aerosols in ECS and more studies are needed to understand the potential effects on air quality and climate of surrounding areas.

10RA.9

Concentrations and Fluxes of Water Soluble Inorganic Aerosol Components above Tropical Rainforest. Robbie Ramsay, Chiara Di Marco, Mathew Heal, Matthias Sörgel, Meinrat O. Andreae, Paulo Artaxo, Alex Araujo, Marta Sá, EIKO NEMITZ, *Centre for Ecology and Hydrology*

The interaction between biosphere and atmosphere in the cycling of gas and aerosol species is of key importance in considering overall emission and deposition rates of nutrients and pollutants. Understanding of the biosphere-atmosphere processes that govern these cycles is critical to modelling global concentrations of atmospheric aerosols and trace gases, which in turn is vital to developing predictions for future climate, air quality and trans-boundary air pollution. However, to understand these processes, more measurements over a variety of different ecosystems are required, preferably measurements which are taken in real time, which are of high temporal resolution and record a variety of species simultaneously and at potentially low background concentrations. In particular, very little is known about the role of biosphere-atmosphere exchange in the nutrient cycling in and above tropical rain forests. While aerosol concentrations can provide information on the regional transport of compounds, fluxes allow an insight into the chemical process in the forest.

In this work, the concentrations and fluxes of water-soluble aerosol species NH_4^+, Cl^-, NO_2^-, NO_3^- and SO_4^{2-} in total suspended particulate (TSP) and their precursor gases NH_3, HCl, HNO_2, HNO_3 and SO_2 were measured using a Gradient of Aerosols and Gases Online Registrator (GRAEGOR) above a tropical rainforest site located at the Amazon Tall Tower Observatory (ATTO) in Amazonia, Brazil. Measurements were taken during the dry season from the 4 October to 10 November 2017. From the measured concentration-gradients and ancillary meteorological measurements, fluxes for each species were derived using the hybrid Aerodynamic Gradient Method and the Modified Bowen Ratio Method. Deposition velocities for each species were calculated and compared to theoretical deposition velocities, and interpreted in relation to measurements of leaf wetness at the canopy level.

The average concentrations for aerosol species at each of the measurement heights (42 m and 60 m) throughout the campaign were 0.26/0.26 $\mu g\ m^{-3}$ for NH_4^+, 0.11/0.12 $\mu g\ m^{-3}$ for Cl^-, 0.39/0.48 $\mu g\ m^{-3}$ for NO_3^- and 0.48/0.49 $\mu g\ m^{-3}$ for SO_4^{2-}. The mean concentration values of measured precursor gases were 0.26/0.23 $\mu g\ m^{-3}$ for NH_3, 0.10/0.11 $\mu g\ m^{-3}$ for HCl, 0.06/0.06 $\mu g\ m^{-3}$ for HNO_2, 0.24/0.26 $\mu g\ m^{-3}$ for HNO_3 and 0.20/0.23 $\mu g\ m^{-3}$ for SO_2. The aerosol concentration values were mostly in agreement with previous measurements made at similar time of year, except for higher mass fraction contribution of chloride and nitrate in the current study. This could indicate regional or long-distance transport of coarse chloride (sea salt) and coarse nitrate that previous measurements would not have detected due to their use of a smaller particle size cut-off compared with the one in this study.

10RA.10

Characterization of Aerosol Size Distributions and Optical Properties in the Canadian High Arctic using Surface and Columnar Observations. PATRICK HAYES, Samantha Tremblay, Norman O'Neill, Jai Chaubey, AboEl-Fetouh Yasmin, Rachel Chang, Felicia Kolonjari, Sangeeta Sharma, Richard Leaitch, Pierre Fogal, *Université de Montréal*

This study presents long-term observations of aerosol size distributions for both coarse and fine modes as well as of aerosol light scattering and absorption that are ongoing at the Polar Environment Atmospheric Research Laboratory (PEARL) in the Canadian High Arctic (80N, 86W) since summer 2016. A variety of field measurements are utilised including a scanning mobility particle sizer, an optical particle counter, and two Photoacoustic Extinctiometers. The scattering and absorption coefficients are measured at 405 nm and 870 nm, and from these measurements a number of derived parameters are calculated such as aerosol single scattering albedo (SSA), the scattering and absorption angstrom exponents as well as black carbon concentration. The measurements of the aerosol scattering and absorption coefficients are also compared against the coefficient values calculated using Mie theory and the measured aerosol size distribution in an optical closure study.

As expected a strong seasonal variation in scattering and absorption is observed with higher scattering and absorption coefficient values during the wintertime Arctic Haze. Average SSA values of 0.96 are observed for 405 nm and 870 nm during the 2016 winter. The scattering angstrom exponent (SAE) varied between values of 1 and 4, wherease the absorption angstrom exponent (AAE) showed relatively little variation with an average value of 0.83 during the same period. The changes in the SAE are likely due to changes in particle size, with periods of low SAE resulting from long-range transported black carbon and periods of high SAE suggesting larger coated particles, possibly containing black carbon as well. Furthermore, a preliminary optical closure study has shown that the measured scattering coefficient is in agreement with the values calculated using Mie Theory, the measured size distributions, and an assumed value for the refractive index.

Finally, the optical properties determined from the surface measurements will be compared against sun photometer measurements to understand the relationship between the surface and columnar aerosol optical properties. The measurements at PEARL provide a unique combination of surface and columnar data sets on aerosols in the High Arctic, a region where such measurements are scarce despite the impact of aerosols on the climate of the Arctic.

10RA.11

Chemical Composition of Ultrafine Particles in the Amazon Basin During GoAmazon2014/5. HAYLEY GLICKER, James Smith, Scot T. Martin, Suzane de Sá, *University of California, Irvine*

While ultrafine (sub-100 nm diameter) particles have been observed in the Amazon Basin, the chemical processes that lead to their formation are not well understood. This is due to the lack of direct observations of boundary layer new particle formation as well as to the challenges in measuring ultrafine particle physico-chemical properties. The Amazon Basin is a unique environment with a climate that is highly sensitive to perturbations in aerosol particle properties and concentrations.(1) In addition, deforestation and urbanization are rapidly changing the Amazon’s environment, and the influence of these anthropogenic activities on ultrafine particles is largely unknown. This work focuses on characterizing the chemical composition of ultrafine particles and understanding the influence of both natural and anthropogenic sources on nanoparticle formation and growth processes in the Amazon Basin. These observations took place during the Observations and Modeling of the Green Ocean Amazon (GoAmazon2014/5) (2) campaign and feature measurements of ultrafine aerosol particle composition using the Thermal Desorption Chemical Ionization Mass Spectrometry (TDCIMS), as well as comparisons with other ground-based instruments deployed at the T3 site in Manacapuru, Brazil.

Our analysis focuses on a span of twelve days during the wet season, which featured a period with relatively clean air masses and a period with air masses that appear to have passed through Manaus, a large city of 1.8 million people. We identified the presence of compounds, such as 3-methylfuran and other IEPOX fragments, in the particle phase, that are indicators of a biogenic influence on ultrafine particle formation and growth. A fragment of an organic nitrogen compound, which we identify as NCO-, was the most abundant ion observed by the TDCIMS. This ion was also the most abundant ion observed in previous measurements by TDCIMS in a region impacted by emissions from the Mexico City Metropolitan Area. Sulfate was a minor constituent and did not exhibit a diurnal pattern, which suggests a long range transport source. During the period where air masses from Manaus were measured, there was less variability in the diurnal pattern of detected compounds but otherwise no significant difference in ion abundance compared to the clean, background period. The most abundant ions identified in ultrafine particles are compared to the potential sources determined from the analysis of backward trajectories obtained from an air parcel trajectory analysis using the HYSPLIT model.

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10RA.12

Ambient Fine Particle Trace Elements over Van Vihar National Park, Bhopal, India and an Assessment of Associated Potential Health Risks. JAYANT NIRMALKAR, Samresh Kumar, Ramya Sunder Raman, *Indian Institute of Science Education and Research Bhopal*

Ambient $PM_{2.5}$ (fine particles, diameter ≤ 2.5µm) over Van Vihar National Park in Bhopal, Central India were sampled. Samples were collected ever-other-day for two years (01 January 2012 to 31 December 2013) using Mini-Vol® sampler (Airmetrics, OR, USA, 5 LPM, 12 h integrated sampling) on to Teflon filter substrates. The collected aerosol samples were subjected to chemical analysis using Energy Dispersive X-ray Fluorescence to measure the concentrations of 27 trace elements (Mg, Al, Si, S, Cl, K, Ca, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Br, Rb, Sr, Cd, In, Sn, Sb, Hg and Pb). Of these elements, the sum of percent missing and percent below detection limits concentration were found to be more than 60% for Cr, Co, Ni, Se, Br, Cd, Sn, Sb and Hg.

This study presents the temporal variability of trace elements measured at the study site. Amongst all measured elements, the top contributor was S (2.7 μgm^{-3}) followed by Si (1.3 μgm^{-3}) and Al (1.1 μgm^{-3}). During the study period, the average mass concentration of the sum of crustal elements (Mg, Al, Si, Ca, Ti and Fe) was found to be highest (4.9 μgm^{-3}) during the pre-monsoon season (March April and May) whereas the sum of toxic elements including As, Cd, Hg and Ni and other major trace elements including Cl, K and S were highest at 0.3 μgm^{-3} and 5.7 μgm^{-3}, respectively, during the post-monsoon season (October, November and December). Further, the average mass concentration of the sum of non-exhaust traffic indicators including Zn, Pb, Cu, Sb and Cr was found to be highest (0.5 μgm^{-3}) during the winter season (January and February).

Trace element mass distributions, correlation analysis and other statistical tools together with air parcel trajectory ensemble analyses will be used to understand the likely sources of these species and the geographical source locations/preferred transport pathways. Further, the associated potential carcinogenic and non-carcinogenic health risk from the exposure to these trace elements will also be estimated.

10RA.13

Measurement of Aerosol Flux Using UAV in Goseong, South Korea. Hee-Sang Kim, KANG-HO AHN, Hee-Ram Eun, Yong-Hee Park, Woo-Young Kim, *Hanyang University, R. of Korea*

Aerosol problems have many scientific and visibility, human health, and global climate. There are three factors that have a significant impact on the mass concentration of aerosol: domestic sources of pollutants, external sources outside the country and weather conditions.

Aerosol can know the relationship between the rise and the reduction of up to 1km in the vicinity of various weather conditions on the ground, that impact on wind.

In this experiment, we can observe many fine dusty days and few fine dusty days.

10RA.15

Single Particle Analysis of Samples Collected During the Actris-2 Field Campaign at the Mt. Cimone Station. TYLER CAPEK, Swarup China, Daniel Veghte, Angela Marinoni, Douglas Orsini, Claudio Mazzoleni, *Michigan Technological University*

Atmospheric particles influence the Earth's radiative balance directly by scattering and absorbing solar radiation and indirectly by affecting the formation of clouds and altering the overall albedo of clouds. Due to many socio-economic and environmental reasons, the Mediterranean region is considered a hot spot for climate change and air quality issues. In July 2017 we measured the optical properties and collected samples of atmospheric particles at Monte Cimone as part of an Aerosol Cloud and Trace Gases Research Infrastructure (ACTRIS-2) field campaign. Monte Cimone, the highest mountain in the northern Apennines of Italy, is ideally situated to study the physical and chemical properties of atmospheric particles in the Mediterranean free troposphere as well as the heavily polluted Po Valley (just to the north).

Atmospheric particles ranging in aerodynamic diameter from 0.25-1µm were collected using a 4-stage cascade impactor from the O. Vittori Observatory near the summit of Mt. Cimone. We utilized scanning and transmission electron microscopy coupled with energy-dispersive X-ray spectroscopy (EDS) to determine the abundance, morphology, elemental composition, and mixing state of single particles. We determined the abundance of size-resolved particle classes from the elemental composition of numerous particles. Furthermore, we performed dynamic hydration experiments using an environmental SEM to study the hygroscopic behavior of different particle classes. We observed a considerable fraction of aged sea-salt, sulfates, calcium-rich dust particles, and other carbonaceous particles such as soot and tar balls. On July 19th, 2017 the microscopy analysis showed that 15% of the atmospheric particles were tar ball aggregates, a carbonaceous particle typically associated with biomass burning. Our results indicate that biomass burning plumes and marine sources influenced the air masses sampled at the station. This study provides information on the morphology and composition of single particles at high altitudes where this kind of data is scarce. The results can enhance the understanding of the optical properties of aged particles.

10SA.1

Use of Specific Primary and Secondary Organic Markers for PM Source Apportionment Based on Positive Matrix Factorization (PMF). Deepchandra Srivastava, Olivier Favez, Emilie Perraudin, Jean-Luc Besombes, Franco Lucarelli, Laurent Alleman, Grazia Maria Lanzafame, Sophie Tomaz, Jean-Luc Jaffrezo, Benjamin Golly, Nicolas Bonnaire, Valerie Gros, Eric Villenave, ALEXANDRE ALBINET, *INERIS*

Organic aerosol constitues a major part of particulate matter (PM) accounting for about 20-60% of the total mass. OA is still poorly understood due to the complexity and the diversity of the PM sources (anthropogenic and biogenic) and processes involved (primary and secondary). The aim of this work was to refine the PM source apportionment using specific primary and secondary organic molecular markers. Field measurements were performed at both locations in France (Grenoble, 2013 and at the SIRTA station, 2015 (25 km SW from Paris)) over 1 year with PM_{10} samplings, every third day. Intensive observations at SIRTA have been also performed with PM_{10} samples collected every 4-hour during a period of severe PM pollution event (PM>50 µg m-3 for several days) in March 2015. Following an extended chemical characterization (from 139 to 216 species quantified), the use of key primary and secondary organic molecular markers in positive matrix factorization (PMF) model allowed to deconvolve 9 and 11 sources (Grenoble and SIRTA, respectively), including common ones (biomass burning, traffic, dust, sea salt, secondary inorganics and nitrate), as well as uncommon resolved sources such as primary biogenic OA (fungal spores and plant debris), biogenic SOA (marine, isoprene) and anthropogenic SOA (nitro-PAHs, oxy-PAHs, phenolic oxidation). Discussion will further underline the details of the chemical and temporal/seasonal profiles of each source, and their relative contributions. In addition, the high time-resolution filter dataset obtained at SIRTA allowed the study of the diurnals of the identified sources and the better understanding of the chemical processes involved.

10SA.3

Physicochemical Characteristics and Source Apportionment of PM2.5 in an Inland City of Baoji, China. ZHOU BIANHONG, Li Meijuan, Fang Ni, Zhang Zhangquan, Liu Suixin, *Baoji University of Arts and Sciences*

PM2.5 samples were collected from March 2013 to March 2014 in inland city of Baoji, China. The daily and seasonal variations of PM2.5 mass and major chemical components were analyzed. The source apportionments were obtained by using positive matrix factorization (PMF).
The concentrations of PM2.5 was 153.6±90.9 μg•m-3 during the sampling period. The seasonal variation of PM2.5 concentrations followed by the order of winter > autumn > spring > summer. SO42-, NO3- and NH4+ were the major ions, which accounting for 78%-91% of total ions. The concentration of SO42-, NO3- and NH4+ were highest in winter, however, SO42- was also abundant in summer. The seasonal ratio range of NO3-/SO42- is 0.52-0.79, indicating that pollutants are mainly emitted from stationary sources, especially from coal combustion. The seasonal trend of WSOC followed as winter > autumn > spring > summer. OC presented a highest concentration in winter. EC concentrations varied insignificantly in different seasons. Ca, Fe and Zn were the main elements. Ca, Ti and Fe were mainly emitted from natural sources, in contrast to Zn, As, Br and Pb, which were mostly derived by anthropogenic activities. However, Cr and Mn were affected by both natural and anthropogenic emissions. Material balance showed that organic matter (OM) accounts for 20.1%-31.4% of annual PM2.5 concentration, and the contribution of SO42-, NO3- and fugitive dust (FD) were 14.6%- 24.1%, 10.3%-16.3% and 10.3%-24.1%, respectively. OM and FD were the most abundant compositions in spring, accounting for 19.9%-29.4% and 17.9%-26.9% of PM2.5. On the contrast, SO42- was the highest contributor (25.2%-37.4%) in summer. In autumn and winter, PM2.5 was mostly consisted by OM (25.6% to 35.9% and 21.9% - 37.2%). PMF results indicated that the major contribution factors are secondary sulfate (24%), coal combustion (18%), secondary nitrate (16%), biomass burning (15%), fugitive dust (15%) and motor vehicles (12%).

10SA.4

Assessing the PM2.5 Imbalance between a Far and Near-Road Location: High Temporal Frequency Source Apportionment and the Role of Black Carbon. UWAYEMI SOFOWOTE, Robert Healy, Yushan Su, Jerzy Debosz, Michael Noble, Anthony Munoz, Cheol H. Jeong, Jon M. Wang, Nathan Hilker, Greg J. Evans, Philip K. Hopke, *EMRB, Ontario Ministry of the Environment and Climate Change*

The differences in $PM_{2.5}$ concentrations between two adjacent stations, one situated near a major highway and the other much farther were used to develop a protocol for determining the impact of highway traffic on particulate matter concentrations at the roadside. The near-road station was 2.5. This particulate matter difference, formally called the $PM_{2.5}$ imbalance was subjectively defined as a case wherein $|$Near-road $PM_{2.5}$ - Farther from road $PM_{2.5}|$/Near-road $PM_{2.5} \gtrsim 50\%$. Of interest was the variation of factors (sources) obtained from source apportionment analyses of the speciation data from the roadside station during these imbalance events. One of the factors, a black carbon factor was determined to be the major cause of the $PM_{2.5}$ imbalance and was very prominent for the case when $PM_{2.5}$ concentrations at the near-road station were greater than the farther-station $PM_{2.5}$. We then regressed the black carbon concentrations observed during these specific events against other traffic-related and meteorological parameters with nonlinear optimization algorithms in our attempts to model any potential relationships. We noted that the traffic counts of heavy duty vehicles (predominantly diesel-powered) dominated the relationship with black carbon while contributions from light duty vehicles were negligible during these $[PM_{2.5}]_{\text{Near-road}} > [PM_{2.5}]_{\text{Farther}}$ events at the near-road station. This work discusses the most critical ways that highway traffic can contribute to local ambient $PM_{2.5}$ concentrations that commuters are exposed to and should inform policies and strategies for particulate matter pollution reduction at the roadside.

10SA.5

An Improved Approach to Resolve Sources of Organic Aerosol by Combining Offline and Online Ambient Measurements. DEEPCHANDRA SRIVASTAVA, Olivier Favez, Jean-Eudes Petit, Yunjiang Zhang, Uwayemi Sofowote, Philip K. Hopke, Nicolas Bonnaire, Emilie Perraudin, Valerie Gros, Eric Villenave, Alexandre Albinet, *INERIS*

Organic constituents are a major component of ambient particulate matter (PM) and have significant impacts on air quality and climate change. Over the last decade, the use of online instrumentation (i.e. AMS and ACSM) has successfully provided real time measurements of particulate organic fractions as well as information on their sources. However, a full comprehension of organic aerosol (OA) sources is still difficult to achieved due to the complexity and variability of the processes involved. Combining different datasets from several measurement systems to refine the source apportionment of OA, and notably secondary ones (SOA), is probably one of the best way to achieve this goal. In this study, we performed a short term intensive campaign, in March 2015, at the SIRTA atmospheric research observatory, representing the suburban background air quality conditions of the Paris region (25 km SW of Paris) over a period of intense PM pollution events ($PM_{10} > 50$ µg m^{-3} over several days). PM_{10} samples were collected every 4 hours concomitantly with online measurements including ACSM, 7λ Aethalometer, TEOM-FDMS (PM_1 and PM_{10}), NO_x and O_3 analyzers. A novel OA source apportionment approach has been applied by combining online and offline measurements using time synchronization script (positive matrix factorization, PM, using ME-2 engine). The unified matrix, included OA matrix from ACSM and specific primary (e.g., levoglucosan (biomass burning), 1-nitropyrene (traffic)) and secondary organic molecular markers (e.g., 3-methyl,5-nitrocatechol (biomass burning), α-methyl glyceric acid (isoprene)…) from PM_{10} filters with their original time resolution (30 min for ACSM and 4 h for PM_{10} filters). The results obtained allowed the deconvolution of 10 OA factors including 4 different biomass burning sources (primary and secondary OA). The time synchronization provided more information than the conventional PMF approaches based on ACSM or filter data only and allowed a comprehensive description of the atmospheric processes related to the different OA sources.

10SA.6

Particulate matter in the Northwest of the Iberian Peninsula: A one-year study. Fernanda Oduber, Carlos Blanco-Alegre, Ana Isabel Calvo, Amaya Castro, Roberto Fraile, Teresa Nunes, CÉLIA ALVES, *University of Aveiro*

Humans and the environment are exposed to a complex mixture of several atmospheric contaminants, including particulate matter (PM). The study of the PM composition and its temporal variation allows determining the potential emission sources and, therefore, to establish mitigation measures. Researches on the spatial and temporal variation of chemical characteristics of PM in the northwest of the Iberian Peninsula are scarce.

The present study was carried out in León city, located in the northwest of the Iberian Peninsula (42° 36′ N, 05º 35′ W and 838 m above sea level), between 9th March 2016 and 14th March 2017. PM_{10} sampling was carried out on the roof of the Faculty of Veterinary (University of León). Two different devices were used: a) a low volume sampler (TECORA, ECHOPM) operated with 47 mm diameter teflon filters and b) a high volume sampler (CAV-A/Mb) equipped with 150 mm diameter quartz filters. Quartz filters were used to determine PM_{10} by gravimetry, and organic and elemental carbon (OC and EC) by a thermo-optical method. Teflon filters were used for the analysis of water soluble ions (ionic chromatography). Furthermore, an automatic weather station located in the sampling site recorded temperature, wind speed and direction, relative humidity and precipitation data. Likely due to the seasonality of sources and meteorological processes, well-defined temporal differences were observed in PM_{10} concentrations and chemical composition. Monthly and seasonal variations were studied in detail. During the sampling period, the mean temperature and relative humidity were 12 ºC and 64%, respectively. Summer (July-September) was the season with less precipitation and higher mean temperature (21.3 mm and 20 ºC, respectively), whereas spring (April-June) was the rainiest season (223.2 mm). The PM_{10} daily limit value (50 μg/m^3, Directive 2008/50/EC) was only exceeded on 23rd February 2017 (60.4 μg/m^3), coinciding with a Saharan dust intrusion episode. The lowest PM_{10} value (2.0 μg/m^3) was observed in summer, after a precipitation event. Winter (January-March) was characterized by high PM_{10}, OC, EC and NO_3^- mean concentrations (20.6 ± 9.3, 3.0 ± 1.5, 1.0 ± 0.5, and 1.7 ± 1.8 μg/m^3, respectively). These results may be due to the contribution of fossil fuel-based heating systems. The lowest PM_{10} and OC mean concentrations were observed in spring (11.8 ± 6.1, 1.8 ± 1.0 μg/m^3, respectively). The decrease in the particulate matter levels during spring can be associated with the intense precipitation in this period. Summer was characterized by low EC and NO_3^- concentrations (0.6 ± 0.3 and 0.5 ± 0.3 μg/m^3, respectively) and high Ca^{2+} and SO_4^{2-} mean values (0.3 ± 0.2 and 1.6 ± 1.1 μg/m^3, respectively). The presence of high levels of ions, such as Ca^{2+} and SO_4^{2-}, can be attributed to different episodes of African dust intrusions that reached the Peninsula [1, 2].

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10SA.7

Source Apportionment of PM2.5 Using Hourly Measurements of Elemental Tracers and Major Constituents in an Urban Environment: Investigation of Time Resolution Influence. QIONGQIONG WANG, Liping Qiao, Min Zhou, Shuhui Zhu, Stephen Griffith, Li Li, Jian Zhen Yu, *Hong Kong University of Science & Technology*

We demonstrate with field data the benefit of using high-time resolution chemical speciation data in achieving more robust source apportionment of fine particulate matter ($PM_{2.5}$) using positive matrix factorization (PMF). Hourly composition data were collected over a month in Shanghai, including four inorganic ions, thirteen elements, organic and elemental carbon. PMF analysis of the hourly dataset (PMF_{1h}) resolves eight factors: secondary nitrate/sulfate, vehicular/industrial emissions, coal combustion, secondary sulfate, tire wear, Cr&Ni point source, residual oil combustion, and dust, with the first three being the major ones and each contributing to >20% of PM2.5 mass. To characterize the benefit gained from time resolution, we carried out separate PMF analyses of 4-h and 6-h averaged data of the same dataset (PMF_{6h} and PMF_{4h}). PMF_{6h} and PMF_{4h} produce an eight-factor solution sharing similar factors to those by PMF_{1h}, but show less stability and more mixing in source profiles. Profile mixing was especially noticeable for tire wear, coal combustion and Cr&Ni point source in PMF6h, as the 6-h averaging significantly decreased between-sample variability and increased rotational ambiguity. While the three sets of PMF solutions were similar in contributions for factors with major species as source markers (e.g., secondary nitrate/sulfate), larger variations existed for factors with trace species as markers due to mixing of major species in the profiles and higher rotational uncertainties in PMF_{4h} and PMF_{6h}. Our results indicate that hourly time series of elements and major components could achieve more robust source apportionment through better capturing of fast changing dynamics in source activities.

10SA.8

Emission Characteristics of PM2.5 and Trace Gases from Household Wood Burning in Guanzhong Plain, Northwest China. YONG ZHANG, Jie Tian, Junji Cao, Wenjie Wang, Haiyan Ni, Suixin Liu, Zhenxing Shen, *Institute of Earth Environment, Chinese Academy of Sciences*

Considering woods used as the primary fuel on countryside in Guanzhong Plain and its burning contribution for $PM_{2.5}$. Five kinds of common wood fuel (Persimmon tree, Pear tree, Apple tree, Jujube and Peach) were collected and burned in a laboratory combustion chamber with a common stove to determine gaseous pollutants emission (i.e. CO_2, CO, NOx, SO_2) and $PM_{2.5}$ emission with source profiles and speciated emission factors. The average EFs were estimated to be 1401±71 g·kg-1 for CO_2, 53.48±11.83 $g\cdot kg^{-1}$ for CO, 1.48±0.54 $g\cdot kg^{-1}$ for NOx, 0.53±0.19 $g\cdot kg^{-1}$ for SO_2 and 3.01±0.72 $g\cdot kg^{-1}$ for PM2.5. OC, EC and water-soluble ions (sum of Na^+, NH_4^+, K^+, Mg^{2+}, SO_4^{2-}, NO_2^-, NO_3^-, Cl^-) are major constituents for $PM_{2.5}$ mass, accounting for average abundance of 29.86%±2.03%, 15.65%±1.07% and 17.51%±6.24%, respectively. The average EFs of OC and EC were 910±279 mg·kg-1 and 465±279 mg·kg-1. EC1 was the dominant carbon fraction with average abundance of 44%±3% for total carbon in $PM_{2.5}$. For water-soluble ions, Sodium (Na^+), potassium (K^+) and chloride (Cl^-) were the dominant with average abundance of 4.69%±2.51%, 3.81%±2.13% and 3.30%±2.45% in $PM_{2.5}$. Average OC/EC ratio of woods burning was 1.96±0.45, lower than 11.94-20.20 for straw combustion. In addition, the average K^+/EC ratio was 0.25±0.15, an order of magnitude lower than those from straw residues burning (0.65-3.16). Mass reconstruction of PM2.5 could explain average 87.35%±8.28% component. Similarity measures (i.e., Student's t-test, coefficient of divergence) show the wood profiles were similar for the species measured, which indicated those profiles could be resolved from one another by receptor modeling. Woods burning contributed 2.9 $\mu g\cdot m^{-3}$ and 9.8 $\mu g\cdot m^{-3}$ $PM_{2.5}$ in non-hazy day and hazy day in Guanzhong Plain.

10SA.9

Application of Positive Matrix Factorisation to the Source Identification of Pcdd/Fs in Urban Air, South Korea.

EUNHWA JANG, Taewuk Jeong, Nana Yoon, Seungryul Jeong, *Busan Metropolitan Institute of Health and Environment*

Polychlorinated dibenzo-p-dioxins and polychlorinated dibenzofurans (PCDD/Fs) are ubiquitous compounds which produce unintentionally through the chemical manufacturing and combustion processes, persist in the environment and bioaccumulate in the food chain. Because of the known toxic properties of PCDD/Fs, it is required to make an emission estimates for PCDD/Fs to identify the dominant sources to the environment and to examine the effectiveness of source reduction measures.

However, there are considerable uncertainties in making PCDD/Fs emission estimates owing to their source variability. Therefore, source apportionment modeling has been extensively performed to obtain information about site-specific pollution sources using measured concentrations.

Positive Matrix Factorisation (PMF) has been widely applied to ambient measurements in recent years to compare source-specific contributions to atmospheric pollution levels. There are some difficulties to extract site representative profiles because of the uncertainties caused by weathering process (atmospheric reaction and deposition) from each source to receptors. However, the fact that there are distinctive signatures of PCDD/Fs composition among the different sources support the existence of source specific profiles (US EPA, 2006).

PMF 5.0 has been applied to two merged datasets (2 industrial urban sites and 3 urban background sites) consisting of ambient measurements for PCDD/Fs concentrations from 2007 to 2016. An additional industry dataset consisting of both PCDD/Fs and Poly Aromatic Hydrocarbons (PAHs) concentrations informed by knowledge of local emission characteristics has been subjected to PMF to obtain supportive explanations for the PMF factor profiles for PCDD/Fs.

Analysis of industrial urban dataset revealed five major source categories corresponding to industrial thermal processes (accounting for 14.5% of total toxicity equivalent PCDD/Fs mass), ferrous metal production (41.0%), nonferrous metal production (18.6%), diesel vehicle emissions (20.2%) and traffics (5.7%). As expected, metallurgical industry was the dominant contributor to the sum of PCDD/Fs, followed by diesel exhaust emissions. PMF factor profile with emissions from ferrous production activities was predominantly associated with penta- and hexa-chlorinated furans having relatively large toxic equivalence factors.

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10SA.10

Influence of Future Emission Reductions on Source Apportionment of Organic Aerosol in the Houston Region.

BONYOUNG KOO, Alan Dunker, Greg Yarwood, *Ramboll*

Organic aerosol (OA) accounts for a significant fraction of atmospheric fine particulate matter (PM) mass. OA can be directly emitted into the atmosphere (primary OA, POA) or formed secondarily from hydrocarbon precursors (secondary OA, SOA). SOA yields are modulated by concentrations of NO and SO_2 which have anthropogenic sources that change in response to our activities and policies. NOx has direct and indirect effects on SOA formation: a direct effect is that SOA yields depend on NOx; an indirect effect is that species which oxidize hydrocarbon precursors to SOA (e.g., OH and NO_3 radicals) also depend on NOx. Therefore, accurate source apportionment of SOA requires a methodology that properly takes into account both the direct and indirect effects. Tagged species methods currently available in photochemical grid models do not account for the indirect effects. A recently developed source apportionment approach called the Path-Integral Method (PIM) provides rigorous source contributions by integrating the first-order sensitivity of pollutant concentrations to emissions computed at several emission levels. The PIM can be applied for any species included in the chemical mechanism, has a mathematically rigorous methodology, and allows the numerical accuracy of the method implementation to be checked for each application. The PIM has been successfully used to compute source contributions of gaseous pollutants such as ozone, NO_2 and aldehydes. Here, we apply the PIM to determine contributions of US anthropogenic source sectors to OA in the Houston, Texas region, accounting for both direct and indirect effects of NOx emissions on SOA formation. Two emission scenarios (2013 base year and 2028 projected future year) are used to examine how future emission reductions influence the source apportionment of OA in the region.

10SA.11

Impacts of Hazardous Metals and PAHs in the Ambient Air from Local and Regional Sources and Exceeded Cancer Risks in Taipei city. CHIN-YU HSU, Shih-Min Wang, Tzu-Ting Yang, Jyh-Larng Chen, Hung-Che Chiang, Yuh-Shen Wu, Yu-Cheng Chen, *National Health Research Institutes, Taiwan*

This study assessed the influence of health risks for ambient PM2.5-10- and PM2.5-bound metals/PAHs in terms of the long-range transport in New Taipei City. Particle measurements were conducted during winter and summer in 2014. Twenty-two trace metals and PAHs in PM10 and PM2.5 were analyzed using ICP-MS and GC-MS. Trajectory statistical methods combined with potential source contribution function (PSCF) were utilized to distinguish local and long–range transport of PM concentrations. The positive matrix fraction (PMF) were applied to quantify potential sources of toxic metals/PAHs. The annual mean concentration of PM2.5 was 22.69±9.53 µgm-3, while PM2.5-10 was 19.24±11.08 µgm-3. The level of excess cancer risks for PM2.5-bound metals (6.23×10-5) was higher than those for PM2.5-10-bound metals (1.41×10-5). PM2.5-bounded BaPeq concentrations and cancer risk were respective 0.64±0.34 ngm-3 and 5.59×10-5. A seasonal variation for PMs and most metals/PAHs with a higher level in the winter than the summer were observed. Through a PMF model, the contributors of cancer risk from traffic-related emission (59.75%), coal combustion (20.65%), and re-suspended dust (19.60%) were identified. The enhanced cancer risk due to long-range transport from traffic-related emission, coal combustion, and re-suspended dust are about 4.03%, 9.03%, and 1.48%, respectively.

10SA.12

Long-Term Field Observations of Aerosol Chemical Composition in the Boreal Forest. LIINE HEIKKINEN, Mikko Äijälä, Matthieu Riva, Krista Luoma, Tuukka Petäjä, Douglas Worsnop, Mikael Ehn, *University of Helsinki*

In the past decades the atmospheric fine particulate matter (PM) concentrations have caught attention due to the impacts on climate, health and visibility. Atmospheric aerosols have many sources and they can be directly emitted into the atmosphere as particles or they can be formed from the oxidation of gaseous precursors during new particle formation events. The atmospheric PM loading is greatly enhanced by the partitioning or reactive uptake of gaseous species, where the organics play a key role through secondary organic aerosol (SOA) formation. Biogenic volatile organic compounds (BVOCs) are a major source of SOA especially in regions with dense vegetation. Also anthropogenic emissions have a significant impact on both organic and inorganic PM composition. The aerosol chemical composition greatly impacts both toxicity and the physicochemical properties of aerosols, such as light scattering abilities or hygroscopicity. Therefore, we deployed an Aerodyne Aerosol Chemical Speciation Monitor (ACSM) for a long-term measurement to the BVOC-rich SMEAR (Station Measuring Ecosystem Atmosphere Relations) II station located in the boreal forest in Southern Finland to capture the chemical composition of aerosol particles and its seasonal variation. To understand the true nature of the seasonal variation of the chemical species present in non-refractory submicron PM and detected by the ACSM, a long data sets is crucial to minimize the influence of short-term pollution episodes. In this way, a better understanding of the chemical processes governing the aerosol within the atmosphere is achievable. Therefore, we analyzed a large data set collected from 2012 to 2017 with approximately a 65% data coverage having all the four seasons well represented. The analysis reveals that the chemical composition of aerosol sampled throughout this period, is highly dominated by the organics. Overall this fraction has the highest contribution to the non-refractory PM_1 especially during summer when the BVOC emissions are the highest and the oxidation processes are the strongest within the boreal forest. A more detailed analysis of the organic aerosol composition was carried out by performing positive matrix factorization (PMF) in order to isolate the different sources (e.g. biogenic vs anthropogenic). This mass spectral analysis highlighted a more pronounced anthropogenic influence on the organic aerosol composition during the cold seasons while during the summer the aerosol was mainly biogenic in origin, as expected. In this study, a detailed analysis of the PMF results as well as an analysis of the seasonal variation of both inorganic and organic non-refractory species are presented. The PMF factors were verified and better understood by comparing them to the vast variety of other parameters measured at the SMEAR-II station as well as mass spectra generated from atmospheric simulation chamber experiments. Finally, a robust characterization of the aerosol chemical composition is presented giving a reliable estimation of its true seasonal variation over the boreal forest.

10SA.13

Impact of Environmental Policies and the Economy on Changes in Criteria Air pollutants Concentrations and Particulate Matter Compositions in New York State during 2005-2016. Stefania Squizzato, Mauro Masiol, David Q. Rich, PHILIP K. HOPKE, *University of Rochester, Rochester, 14642, NY, USA*

Over the past several decades, several mitigation strategies have been adopted by federal and state agencies in the United States to improve air quality. These strategies were mostly targeted to reduce SO_2 and NO_x emissions from light- and heavy-duty vehicles and electric power generation. Between 2007 and 2009, the financial/economic crisis also lowered activity and reduced emissions. Simultaneously, changes in the prices of coal and natural gas drove a shift in fuels used for electricity generation toward natural gas.

This study investigates the seasonal patterns, diel cycles, spatial gradients, and trends of gaseous and particulate pollutant concentrations and $PM_{2.5}$ sources over New York State (NYS) between 2005 and 2016. Gaseous pollutants concentrations (SO_2, O_3, CO, and NO_x) and $PM_{2.5}$ mass and chemical speciation data (elements, major inorganic ions, EC, OC) were retrieved from USEPA (https://aqs.epa.gov/api). The final dataset included 54 sites for $PM_{2.5}$ mass and gases (26 for $PM_{2.5}$, 37 for O_3, 26 for SO_2, 8 for NO_x, 2 for NO_y, 11 for CO) and 6 urban sites (Albany, Bronx, Buffalo, Manhattan, Queens, and Rochester) and 2 rural sites (Pinnacle and Whiteface) for $PM_{2.5}$ speciation data.

EPA PMF 5.0 was applied to the speciation data to identify and apportion the major sources of $PM_{2.5}$ across these sites. The relationships between ambient concentrations, changes in emissions retrieved from the national emission inventory (NEI), and economic changes were studied.

Results show that the combined effects of the mitigation strategies, economic pressures, and the recession led to an overall decrease in $PM_{2.5}$ and primary gaseous pollutants concentrations across New York State ultimately resulting in relatively homogeneous spatial distributions for $PM_{2.5}$ and SO_2. $PM_{2.5}$ concentrations decreased significantly at all sites with slopes ranging from -8.6%/y and –2.2%/y. SO_2 concentrations dropped significantly at all sites within this period, with the highest slopes observed at the urban sites (e.g., -8.5%/y at Queens, New York City).

The reduction of NO_x emissions contributed to the reduction of high ozone episodes during summer, but there was no reduction in spring maxima. Increases in autumn and winter ozone concentrations were estimated (e.g., 6.6 ± 0.4%/y on average in New York City). Statistically significant relationships were observed between $PM_{2.5}$, primary pollutants, and economic indicators. Overall, the decrease in electricity generation with coal, and the simultaneous increase in natural gas consumption for power generation, led to a decrease in $PM_{2.5}$ and gaseous pollutants concentrations.

Seven main common sources of $PM_{2.5}$ were identified across the state: (i) secondary sulfate; (ii) secondary nitrate; (iii) gasoline emissions; (iv) diesel emission; (v) road dust; (vi) biomass burning and (vii) OP-rich. A road salt source was identified at Albany, Buffalo, Rochester, Pinnacle and Whiteface. Additional sources at the New York City sites (Bronx, Manhattan, and Queens) were fresh sea salt, aged sea salt and residual oil combustion.

Among the main $PM_{2.5}$ sources, decreases of secondary sulfate, secondary nitrate, and diesel emissions were observed (-6.7±1.1%/y, -5.3±1.2%/y, -5.3±1.9%/y, respectively) across the state. Decreases can be associated with the mitigation strategies aimed at reducing emissions from light- and heavy-duty vehicles and electric power generation and to the shift from high sulfur to ultralow sulfur fuels. Beginning on July 1, 2012, New York State required that all No. 2 oil sold within the state for any purpose to have ultralow sulfur content. Gasoline emissions increased in Albany, Buffalo, and New York City with slopes higher than 7%/y reflecting the increase of registered vehicles in the area (e.g., New York City +9%, Buffalo +5%, and Albany +6% during 2007-2016).

10SA.15

Comparison of Ambient Aerosol Sources at Rural and Suburban Background Sites in Central Europe. OTAKAR MAKEš, Petr Vodička, Jaroslav Schwarz, Vladimír Ždímal, *Institute of Chemical Process Fundamentals of the CAS, v.v.i*

During July and August 2012, and subsequently in January and February 2013, six weeks long intensive measurement campaigns aimed at PM1 ambient aerosol characterization took place at measurement site at Prague - Suchdol. Subsequently similar campaigns took place in National Atmospheric Observatory Košetice at Vysočina highlands. The first campaign took place from January to March 2014 and the second campaign took place from June to August 2014. The Suchdol site, located on the NW outskirts of Prague, was selected as a representative of suburban background station. On the other hand, the Košetice site was chosen as a representative of the rural background station.

The chemical composition and mass concentration were measured by Compact Time-of-Flight Aerosol Mass Spectrometer (C-ToF AMS, Aerodyne) during all campaigns. This measurement was supported by filter sampling, SMPS and trace gases concentrations. Raw data obtained from AMS at 1 minute time resolution were trimmed and averaged over 30 minute intervals. Subsequently, the data included the matrix of concentrations of each mass (*m/z*, mass to charge ratio) over time and the corresponding error matrix were exported for the source apportionment analysis. Data were analyzed using SoFi software (Canonaco et al., 2013), which uses the Multi-linear engine (ME-2) (Paatero, 1999) based on the principle of positive matrix factorization (PMF). The advantage of this approach is that the user may, on the basis of partial knowledge of one or more aerosol sources, limit the number of possible solutions and thus refine the result of the model.

During the summer measurement campaign in Suchdol, the model identified five different aerosol sources. The only identified primary aerosol source was hydrocarbon-like aerosol (HOA) originating from traffic. Semi-volatile oxygenated aerosol (SVOA) was identified as a secondary source of aerosol which is already partially oxidized in the atmosphere. Another source of secondary aerosol was low-volatile oxygenated aerosol (LVOA), which can originate at a large distance from the measuring site. The remaining two identified sources were predominantly inorganic aerosols and were called as SO_4+NH_4 and NO_3+NH_4, where the second mentioned had a very pronounced daily pattern with increased concentrations at night. During the winter campaign in Suchdol, five sources of aerosol were also identified. Probably due to the low temperatures during the day, the model was not able to distinguish the SVOA source. The primary source of biomass burning aerosol (BBOA) from biomass combustion in domestic stoves was newly discovered instead. The situation at Kosetice site was considerably different because the station is not influenced by any town located in the close neighborhood, but it is influenced by the surrounding rural and forest landscape. During the summer, the model distinguished two primary sources HOA and BBOA with relatively low contributions, two secondary sources SVOA and LVOA with a pronounced daily patterns and two mostly inorganic sources SO_4+NH_4 and NO_3+NH_4. In winter, the contributions of both primary sources increased and the SVOA factor was not recognized again.

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10SA.16

Seasonal Variations in Source Apportionment of the Redox Activity of Urban Fine Particulate Matter in Athens, Greece. SINA TAGHVAEE, Mohammad Sowlat, Christopher Lovett, Konstantinos Eleftheriadis, Evangelia Diapouli, Manos Manousakas, Constantinos Sioutas, *University of Southern California*

In this study, we examined possible changes in the compositions and oxidative potential of airborne particulate matter<2.5 µm in diameter ($PM_{2.5}$) at two urban sites in Athens, Greece: an urban traffic (UT) site located in the city center of Aristotelous, and a residential, urban background (UB) site in the outlying neighborhood of Demokritos. We were not only interested in differences between these two sites, but also in changes of PM composition and oxidative potential as the seasons change from summer (July-September) to fall (October-November) to winter (January-March). Chemical and biological analyses were done to determine PM composition and oxidative potential, then source apportionment of the PM redox activity was done using Principal Component Analysis of the chemical components of PM followed by Multiple Linear Regression of the measured oxidative potential on factor tracers (PCA-MLR). PM samples were analyzed for chemical composition, and the dithiothreitol (DTT) and in vitro alveolar macrophage assays were performed to determine PM oxidative potential. Chemical analysis was done for metals, water-soluble organic carbon (WSOC), elemental and organic carbon (EC/OC), organic compounds, inorganic ions, and markers of biomass burning (e.g. levoglucosan). To examine changes in the source apportionment of PM oxidative potential during different seasons, we first conducted a bivariate correlational analysis of the compositional and oxidative potential data to calculate Spearman’s rho coefficients. The correlational data indicating associations between PM components and oxidative potential were then used to perform PCA-MLR in apportioning the measured oxidative potential to distinct source groups and compositional source factor scores. Our findings revealed that the oxidative potential of urban traffic PM was much lower than urban background PM, and the major source contributors to this redox activity were vehicular traffic at the UT site, which was increased during the longer daylight hours of summer that enhanced photo-oxidation of PM, and biomass burning at the UB site, which was enhanced during the winter period.

10SA.17

PM2.5 Source Apportionment Using a Hybrid Environmental Receptor Model. LUNG-WEN ANTONY CHEN, Junji Cao, *University of Nevada, Las Vegas*

Receptor model is an important tool for air quality management. Since none of the modeling approaches is without biases or uncertainties, a weight-of-evidence (WOE) approach that takes into account multiple model results is strongly recommended in practice. This paper introduces the hybrid environmental receptor model (HERM) that can perform EV-CMB and PMF, two most popular receptor models for PM2.5 source apportionment, using a unified algorithm and evaluates it with simulated and real-world datasets. The current HERM software is capable of 1) conducting EV-CMB analysis for multiple samples in a single iteration; 2) calculating EV-CMB and PMF source contributions as well as middle grounds (hybrid mode) between the two; 3) reporting source contribution uncertainties and sample-/species-specific fitting performance measures; 4) interfacing with MS Excel® for convenient data inputs/outputs and analysis. HERM allows a hybrid mode that takes partial source information such as incomplete source profiles available for the region of study to pursue a middle ground between EV-CMB and PMF. This is particularly useful since the inclusion of only reliable source profiles in the model avoids poor fitting in EV-CMB while decreasing the rotational degree of freedom in PMF analysis. HERM implements the constraints differently from the PMF software (e.g., EPA PMF5.0) in that it uses source profile uncertainties explicitly in the effective variance fitting. Initial testing with simulated and real-world PM2.5 datasets show that HERM reproduces exact EV-CMB results from existing software (EPA CMB8.2) but with more tolerance to collinearity and better uncertainty estimates. It also shows that partial source information helps reduce rotational ambiguity in PMF, thus producing more accurate partitioning between highly correlated sources. Moreover, source profiles generated from the hybrid mode can be more representative of the study region than those acquired from other regions or calculated by PMF with no source information. When practicing receptor modeling, users are recommended to first determine the possible number(s) of sources by examining the dependence of fitting performance (χ^2) on source number. HERM in different modes (EV-CMB, hybrid, and PMF) should be carried out with their results compared and reconciled to support the WOE approach of source apportionment.

10SA.18

Impact of Emissions from Ports of Los Angeles and Long Beach on the Oxidative Potential of Ambient PM0.25 Measured across the Los Angeles County. AMIRHOSEIN MOUSAVI, Mohammad Sowlat, Farimah Shirmohammadi, Sina Hasheminassab, Andrea Polidori, Martin Shafer, James Schauer, Constantinos Sioutas, *University of Southern California*

In the current study, we carried out weekly ambient $PM_{0.25}$ sampling in three contrasting sites located at Los Angeles (USC), north Long Beach (NLB), and Port of Long Beach (PRT) to investigate the chemical composition and oxidative stress as well as sources that are contributing to $PM_{0.25}$ in the locations. Measurements took place during June-July of 2017 to partially avoid the formation of secondary origin organic particles. To assess the impact of emissions from ports of Los Angeles and Long Beach on the oxidative stress of ambient $PM_{0.25}$ in different sites, an in vitro cell-based alveolar macrophage (AM) assay was used to quantify the pertinent levels of oxidative potential. Additionally, detailed chemical analyses were also performed to evaluate the chemical components of $PM_{0.25}$ collected at each site. To connect the oxidative potential of the ambient $PM_{0.25}$ to the major sources impacting the three locations, two different approaches were used: (1) a molecular marker-based chemical mass balance (MM-CMB) analysis to apportion the sources that contribute to $PM_{0.25}$; and (2) a principal component analysis combined with multiple linear regression (PCA-MLR) approach to link source factors and individual species to the measured oxidative potential of $PM_{0.25}$. With respect to all the sites, results revealed that vehicular emissions are the dominant source (60%±4%) followed by road dust (10%±3%), and ship emissions (7%±2%). Further, relatively higher shares of secondary organic aerosol (SOA) were found at the receptor sites (33%±4% at NLB and 35%±3% at USC) as opposed to the PRT site (8%±1%). Moreover, oxidative potential induced by ambient $PM_{0.25}$ was also primarily impacted by mobile sources among all sites (with an average contribution of 50%±5%), followed by ocean-going vessel (OGV) emissions near the port terminals (33%±2%) and secondary organic aerosol (SOA) in central Los Angeles (49%±2%). OGV emissions were more pronounced in the oxidative potential of $PM_{0.25}$ at the port terminal area in comparison to the central Los Angeles which highlights the superlative importance of vessel emissions-originated $PM_{0.25}$ in the vicinity of ports of Los Angeles and Long Beach. Our results indicate a 35%±3% decrease from 2007 to 2017 in $PM_{0.25}$ concentrations due to the implementation of the Clean Air Action Plan (CAAP) by the San Pedro Bay Ports executives in 2006.

10SA.19

Strontium and Lead Stable Isotopes as Tracers of PM2.5 in Northern India. RACHEL YORK-MARINI, Swati Sharma, Gazala Habib, Brian Majestic, *University of Denver*

The World Health Organization's 2006 Air Quality Standards recommend a 24 hour mean concentration of 25 µg/m^3 for PM$_{2.5}$. On January 1, 2018, Delhi, India surpassed these guidelines with PM levels of 431 µg/m^3. While vehicular emissions are one of the leading sources of pollution in Delhi, smaller dust particles may be transported from the nearby Thar Desert and contribute to PM$_{2.5}$ concentrations in Delhi. Strontium and lead stable isotopes, which are highly specific to unique geographical areas, along with trace element composition, are ideal metrics to source dust in atmospheric PM. Here, we use these isotope systems to understand whether the nearby Thar Desert is an important dust source for Delhi and Jaipur. We collected PM$_{2.5}$ from two cities in the northern Indian plains: Delhi and Jaipur, India between June and December 2015. This included both the monsoon and non-monsoon seasons. Additionally, soil samples were collected from both cities and from the Thar Desert, and were resuspended to PM$_{2.5}$. All PM and soil samples were acid digested and analyzed for 35 trace elements via ICP-MS. The remainder of the digests were used to measure strontium and lead isotopic composition via MC-ICP-MS, for the purposes of dust tracing.

Elemental composition varied between Delhi and Jaipur, with many trace elements in Jaipur having lower concentrations than Delhi. Trace elements Sn, Zn, Cr, Ni, Sb, and As had concentrations of 0.143, 0.172, 0.010, 0.006, 0.0034, and 0.0015 µg/m^3, respectively, in Delhi and 0.0017, 0.336, 0.0018, 0.0025, 0.0011, and 0.001 µg/m^3, respectively in Jaipur. The dominant elemental components of the PM in Delhi were crustal elements Al, K, Ca, and Fe with average concentrations of 0.788, 0.445, 0.431, and 0.541 µg/m^3, respectively. In Jaipur, crustal elements Al, K, Ca, and Na with average concentrations of 0.593, 0.326, 7.691, and 0.446 µg/m^3, respectively, were the dominant sources of PM. The Delhi PM$_{2.5}$ samples had an ^{87}Sr/^{86}Sr average ratio of 0.7165 ± 0.0012 (uncertainties = +/- 1 standard deviation of all data). Delhi and Thar soil samples had an average ^{87}Sr/^{86}Sr ratio of 0.7155 ± 0.0015. The Jaipur aerosol samples had an average ^{87}Sr/^{86}Sr ratio of 0.720 ± 0.012, while the Jaipur soil samples had an average of 0.7195 ± 0.0006. The results of ^{87}Sr/^{86}Sr ratios and 1/Sr µg/g indicate that strontium in Delhi is coming from multiple sources. Delhi and Jaipur aerosol samples had an average ^{207}Pb/^{206}Pb ratio of 0.893 ± 0.005 and 0.8888 ± 0.0025 respectively, whereas the Delhi and Thar Desert soils had an average ^{207}Pb/^{206}Pb ratio of 0.833 ± 0.009 and Jaipur soils had an average ^{207}Pb/^{206}Pb ratio of 0.8379 ± 0.0018. This, along with no linear correlation between thallium and lead, indicates the source of lead is anthropogenic.

10SA.20

Temporal Variability of Submicron Organic Aerosol PMF Factor Mass Spectra During the Houston Aerosol Characterization and Health Experiment. NANCY SANCHEZ, Henry Wallace, Benjamin Schulze, Rivkah Gardner-Frolick, James Flynn, Barry Lefer, Robert Griffin, *Rice University*

Factor analysis techniques such as positive matrix factorization (PMF) have been widely applied to deconvolute submicron organic aerosol (OA) concentrations observed at multiple urban and rural locations. Despite the extended use of this method, PMF-based OA source apportionment has potential limitations associated with the underlying model assumption of constant PMF factor mass spectral profiles. As OA is emitted and formed in the atmosphere, continuous chemistry (i.e., aging and atmospheric processing) and varying environmental conditions (e.g., temperature and relative humidity) are expected to impact its chemical and physical character over time. The time evolving nature of OA suggests that PMF factors with invariant mass spectral signatures reflect a time average PMF factor composition, which might not fully capture the dynamics of OA character and contributing emission sources during field studies, leading, for instance, to large model residuals during certain sampling periods.

In this study, the degree of variation of OA PMF factors mass spectral signatures and its significance as a potential limitation of PMF analysis have been evaluated by analyzing non-refractory submicron OA concentrations measured in the Houston area during the 2013-2015 Houston Aerosol Characterization and Health Experiment (HACHE). As part of the HACHE study, an Aerodyne high-resolution time-of-flight aerosol mass spectrometer was deployed in a mobile air quality laboratory, and stationary sampling was conducted at over twelve locations across the Houston area with data collection spanning between two and four weeks for each location.

Different continuous and discontinuous time segments of OA mass-resolved concentrations at distinct HACHE sampling sites were analyzed by independent PMF modeling. The O:C and H:C elemental ratios of the different factors in each time-segmented model were determined and their diurnal variation was established. Inter-comparison of the resulting PMF factor mass signatures of the different time-segmented models was conducted based on different similarity metrics including the spectral contrast angle (θ) and the mass/intensity weighted cosine. This comparison indicated significant differences between the mass spectral profile of PMF factors identified as semi-volatile oxygenated, biomass burning and cooking OA (COA) at different time intervals (θ exceeding 20° for most time intervals). Less variability was generally observed for the mass signature of PMF factors classified as low-volatility oxygenated and hydrocarbon-like OA (HOA) in the distinct time segmented models (θ usually below 10°).

Marked differences in the mass spectrum of COA at different time segments were particularly evident for the data under analysis, indicating potential large variation of the sources and dynamics of this aerosol component. Detailed analysis of the COA mass spectral signatures provided insight into the specific character of this factor at different time intervals and allowed its sub-classification as less and more oxidized COA. Although similarity metrics indicated a consistent mass spectrum for factors such as HOA, the differing abundance of specific gasoline and diesel-related oxygenated mass fragments at the different time-segmented models revealed important differences in the character of this factor, indicating that even for factors with highly similar mass spectra, PMF analysis on a time-segmented basis would allow better discerning the variability in the contributions of different sources to the observed OA concentrations at specific locations (e.g., diesel vs. gasoline vehicle emissions).

The results of this study suggest that as significant temporal variation in the mass spectral profiles of the PMF factors is likely to occur, the application of PMF to lumped OA concentration data might be insufficient to reveal the dynamic character of the different OA fractions. PMF analysis of specific time segments could overcome this limitation.

10SA.21

Investigation of Seasonal Sources of Secondary Organic Aerosol in Switzerland Using Extractive Electrospray Ionization Time-Of-Flight Mass Spectrometry (EESI-TOF). GIULIA STEFENELLI, Veronika Pospisilova, Felipe Lopez-Hilfiker, Kaspar Rudolf Dällenbach, Martin Rigler, Christoph Hueglin, Yandong Tong, Urs Baltensperger, Andre S.H. Prévôt, Jay G. Slowik, *Paul Scherrer Institut*

Anthropogenic and biogenic emissions contain large amounts of volatile organic compounds (VOCs) which may undergo photochemical aging to yield secondary organic aerosol (SOA). The magnitude of SOA production from different sources remains highly uncertain, hindering the estimation of the contribution of these sources to the total ambient organic aerosol. Measurement techniques with high time resolution and chemical specificity are thus urgently needed. PSI has recently developed a novel extractive electrospray ionization time-of-flight mass spectrometer (EESI-TOF), which enables real-time chemical analysis of atmospheric particles without thermal decomposition or ionization-induced fragmentation. We present results from the first field deployments of the EESI-TOF. Measurements were performed during summer 2016 at a well-characterized urban site in Zurich and subsequently in the Swiss alpine valley (Magadino) during winter 2017. Positive matrix factorization (PMF) analysis of EESI-TOF data yielded several organic aerosol factors related to primary and secondary emissions. Factors were separated according to different mass spectral fingerprints and aging processes. Some of the retrieved factors correlated strongly with reasonable counterparts from AMS PMF analysis while others provided previously inaccessible insight into sources and ambient processing. Primary factors related to cooking processes, traffic and cigarette smoke emissions were obtained. The retrieved secondary factors during summer in Zurich were strongly influenced by biogenic emissions, and exhibited significant day/night differences. Factors dominating during daytime showed predominantly ions characteristic of monoterpene and sesquiterpene oxidation while the night-time factor included less oxygenated and more volatile terpene oxidation products, as well as organonitrates which were likely derived from NO3 radical oxidation of monoterpenes. These results contrast with measurements in a Swiss alpine valley during winter, where wood burning emissions were dominant and the retrieved factor mass spectra are compared to spectra generated from smog chamber aging of emissions from residential wood burning appliances.

10SA.22

Assessment of Residential Wood Combustion Influences on Air Quality in a Suburban Area From Eastern Europe.

LUMINITA MARMUREANU, Cristina Marin, Alexandru Dandocsi, Simona Andrei, *National Institute of R&D for Optoelecttronics*

Atmospheric aerosols represents an important component of the Earth System. The aerosol various effects on climate still remain nowadays weakly understood. Biomass Burning aerosol represent one of the most abundant aerosol during cold season especially in the regions with winters dominated by negative values. Biomass burning (BB) aerosols plays a major role in different aspects of weather, climate and atmospheric chemistry. Biomass burning has an important contribution to the total concentration of the Black Carbon (BC) and to the organic aerosol present into the atmosphere. The organic aerosols represent one of the most important fractions of the total aerosol. Until now important researches focused on the assessment of the BB aerosol fraction of the total PM were made across the Europe underlining their impact, especially during winter. Even so, the Eastern Europe represents one of the important area less covered by research in the recent years. The influence on fine aerosol levels produced by residential heating in a periurban environment (Romania) was investigated during winter period. High-time resolved data on light-absorbing aerosols using seven-wavelength Aethalometer and submicronic organics derived from ACSM were combined during dedicated sampling winter campaigns carried on in cold seasons starting from 2015 to 2017. The measurements were made in a periurban area near Bucharest highly influenced by residential heating during the cold season. The main sources of heating in this area are represented by pellets, wood and natural gas. High impact of residential heating can be noticed, the BC resultant from biomass burning having an influence that frequently overpass 45% from total equivalent BC, and for significant periods of time representing the dominant fraction. The results were correlated with markers for fresh BB derived from ACSM (aerosol chemical speciation monitor) data (m/z 60, 73) specific to ”levoglucosan like" anhydrosugar produced by cellulose pyrolysis. The positive matrix factorization was applied to organic spectra, the BBOA (biomass burning organic aerosol) representing an important fraction of winter time period. The BC and submicron organic particle measurements conducted for almost 9 winter months shows a variation of chemical composition of submicron non-refractory aerosols interlinked with specific meteorological parameters. Different diurnal patterns can be noticed for BC characteristic for fossil fuel different than BC resulted from wood burning. The diurnal pattern of Biomass Burning aerosol show maximum in the afternoon with and minimum during noon time, but also significant contribution during entire night time.

10SA.24

Estimation and Sources of Cloud Water SO4 and NO3 Aerosols from Rainwater over High Altitude Station. YANG LIAN, P.S.P. Rao, G. Pandithurai, *IITM, Pune*

Western Ghats act as a hilly barrier for the monsoon clouds and it facilitates cloud dynamics by its orography, but aerosol composition and size play an equally major role into the cloud microphysics and their development, therefore in this present study an attempt has been made to estimate the aerosol mass concentration into the cloud. High altitude cloud station at Mahabaleshwar gives us a new opportunity to explore these relations during monsoon, as warm cloud touches to the ground here. Using multiple in-situ instruments, first time over the Western Ghats, we estimated the concentrations of SO4 and NO3 from rainwater into the cloud water by approximating wet scavenging percentage between 10-30% for initial and final phase rainfall from ACSM and source-apportioned three major contributing sources such as Vehicular, Thunder Lightning, and Long-range transport. The Lightning Location Network and CWT analysis result show that during the initial phase of monsoon collected rainwater, the aerosol composition of SO4 and NO3 are mostly affected by local and thunder lightning emissions whereas at departure phase collected rainwater mainly being influenced by local and long-range transport from Metropolitan city (Mumbai).

Keyword: Rainwater, Scavenging, Aerosols, CWT, Monsoon, Source-apportioned

10SA.25

Long-term Characterization and Source Apportionment of Carbonaceous Aerosols over Five Sites in Northern India.

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Carbonaceous aerosols form a major fraction (up to 90%) of fine mode particulate matter (PM2.5) and have important but highly uncertain implications for air quality, climate and human health. Therefore, identification and quantification of elemental and organic carbon sources is important to design effective mitigation strategies. In this context, PM2.5 filter samples are collected twice a day during first quarter of 2018 and bi-weekly during the rest of the year at five sites spreading upwind (sub-urban) and downwind (urban) of New Delhi.

New Delhi is typically situated 160 Km south of Himalayas and in close proximity to the Thar Desert. It is surrounded by the adjoining state of Haryana on three sides (North, West and South) and experiences prevailing north westerly winds from Himalayas sweeping the northern Plain during winter and south westerly winds during summer and monsoon (travelling from Arabian sea) and spring season affected by south west winds. To understand the effect of local and regional transport of the pollutants in the capital city, one upwind site in north west direction (IITM Hisar, Haryana), three sites in Delhi (North west: IITM, South west: IITD and South east: MRIU) and one downwind site in South east direction have been chosen. IITM Hisar is a sub-urban north western part of Haryana with moderate to high industrial activity (e.g. steel plants situated on periphery of the city). IITM is a central urban part of Delhi, surrounded by forest area and residential colonies. On the other hand, IITD is more of an urban residential site surrounded by moderate traffic density roads (~200 m away). Further, MRIU is also a residential campus in close proximity to the main road with both heavy and light heavy duty vehicles. Being a part of long mountain range (~692 Km) extending towards South west of the sampling site, it experiences humid subtropical and hot semi-arid continental climate similar to the upwind site. Further, extending to ~600 Km in South east direction is the next urban sampling site (IITK), which is also a residential campus with heavy traffic road in the close proximity of ~200 m and upwind of a coal power

In this study, the re-aerosolized filter extracts are analyzed by a newly developed and extensively used offline- aerosol mass spectrometer (AMS) method and extended to a novel extractive electrospray ionization long-time-of-flight (EESI-LToF) mass spectrometric technique. The resulting mass spectra are analyzed by positive matrix factorization implemented within the multilinear engine and Source Finder (SoFi) interface. Coupled with radiocarbon (14C) and major ion analysis, this approach will provide an unequivocal separation of fossil (traffic exhaust and coal burning) and non-fossil (biogenic emissions and biomass burning including heating and open fires of agricultural and other wastes) in both primary and secondary organic aerosol (SOA). Application of this analysis to a long-term dataset collected across five sites yields a spatially and temporally comprehensive overview of the predominant sources affecting New Delhi air quality. We expect that the potential outcomes of this study will help in constraining the potential primary and secondary organic as well as inorganic aerosol sources, facilitating the development of efficient control measures to control local and regional emission sources.

10SA.26

Responses of Aerosol Mass Spectra to Temperature Related Tree Stress. KRISTINA PLAUSKAITE, Julija Pauraite, Steigvile Bycenkiene, Algirdas Augustaitis, Vitas Marozas, Gintautas Mozgeris, Vidmantas Ulevicius, *SRI Center for Physical Sciences and Technology*

Biogenic secondary organic aerosol (BSOA) formation from biogenic volatile organic compounds (BVOC) oxidation affects the chemical and physical properties of the atmosphere. BVOCs emitted by trees in response to temperature related abiotic stress influence high levels of BSOA compounds. Therefore, the objectives of this study were to quantify the temperature-response effect on forest BSOA on purpose to gain more insights in the *m/z* ratios and to investigate the relation of BSOA concentration and the changes in tree trunk circumference. The chemical composition of atmospheric aerosol particles (PM1) was characterized using a high-resolution aerosol chemical speciation monitor (ACSM, Aerodyne Research Inc., USA) at forest site station in the eastern part of Lithuania (55.46º N, 26.00º E, 160 m above sea level) during two investigation periods: August - October (2013) and July – September (2016). Tree trunk circumference was measured during the period of May – September, 2016 using a logging band dendrometer (DRL26), which was fixed to the trunk of 3 Scots pines (*Pinus sylvestris* L.) and 3 Norway spruces (*Picea abies* Karst.). The scale of growing rate indicates the number of millimeters increased after the beginning of measuring campaign. The concentration and chemical composition of PM1 depends on the air mass types advecting the measurement site, meteorological factors and solar radiation. To identify events of clean air masses advection the analysis of 72-h air mass backward trajectories at a height of 500 m above model ground level was performed using the Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model.

During the investigation period, the mass concentrations of ammonium, nitrate, sulphate and organic species were evaluated. Contribution of organics to PM1 was dominant and reached 69% (5.75 μg/m^3 (SD=5.73 μg/m^3)) of the total loading. The mass concentration of the sulphate compound was significantly lower (1.39 μg/m^3 (SD=1.83 μg/m^3)) and contribution to the total loading was 17%. The average mass concentrations of nitrate and ammonium were 0.50 μg/m^3 (SD=0.67 μg/m^3) and 0.63 μg/m^3 (SD=0.92 μg/m^3), respectively. Such chemical composition of PM1 demonstrates low influence of anthropogenic sources at the investigation site. Three organic aerosol (OA) factors were distinguished by positive matrix factorization (PMF) analysis applied for the ACSM data: oxygenated OA (OOA), hydrocarbon-like OA (HOA) and biomass burning OA (BBOA). For distinction of BBOA and HOA factors external profile references were used with a values equal to 0.5 and 0.1, respectively. The concentration of BBOA was low (1.83 μg/m^3 (SD=2.23 μg/m^3)) and its contribution to the total OA mass concentration was only 30%. Likewise, the contribution of HOA to the total OA mass concentration was only 5% with the average mass concentration of 0.33 μg/m^3 (SD=0.38 μg/m^3). Thus, the PMF analysis revealed a minor influence of anthropogenic factors. The normalized mass spectrum was calculated for comparison of aerosol mass spectrum at the high and low temperatures. It has been found that the *m/z* signals from 30 to 149 were higher during the days with high temperatures and the signal intensities of five *m/z* (42, 43, 45, 53 and 59) were about 2.1 – 2.7 times higher during these days. These *m/z* signals could be considered as possible "markers" indicating stress-induced changes in BSOA formation. For the further investigation of temperature influence on tree stress related organics concentration, the submicron forest organic aerosol (SFOM) concentration was calculated. Stress response analysis confirmed that SFOM increases exponentially with temperature and that shrinkage of tree trunk circumference might be observed through enhancement of the *m/z* signals.

10SA.27

Influence of Traffic Emissions on Chemical Composition of Particles in Helsinki, Finland. MINNA AURELA, Kimmo Teinilä, Sanna Saarikoski, Jarkko Niemi, Harri Portin, Pasi Aalto, Liisa Pirjola, Hilkka Timonen, *Finnish Meteorological Institute*

Particle emissions from traffic are known to significantly contribute to regional air quality and the Earth's radiation budget. Particulate matter (PM) emission categories for traffic has been estimated to be 27% in the Helsinki metropolitan area in Finland. Primary particles emitted from motor vehicles consist mainly black carbon and organic material, but motor vehicle emissions include also gaseous compounds like volatile organic compounds, which may produce secondary particles. In order to reduce PM concentrations and improve urban air quality, detailed information on PM concentrations, chemical composition and the contribution of local sources to PM is needed.

The concentration and chemical composition of submicron PM were measured in Helsinki from August 2016 to May 2017 simultaneously at two urban locations: at the urban background site (SMEAR III) and at the curbside in a street canyon (Supersite). The SMEAR III, is located on a small hill, approximately 150m away from one of the main streets (43 000 vehicles/working day) leading to city center. The other station, Supersite, is located in a street canyon on the sidewalk next to another main street (28 000 vehicles/working day) leading to the city center. The chemical composition of non-refractory submicron particles (NRPM1: organic aerosol (OA), sulfate, nitrate, ammonium and chloride) was measured in-real time with an aerosol chemical speciation monitor (ACSM). An aethalometer or a multi-angle absorption spectrometer were used for black carbon measurements. In addition, particles number size distributions and concentrations of trace gases were measured. The mass to charge ratio (m/z) of 55 and 57 and their ratio to total OA, f55 and f57, respectively, were used for estimating the contribution of traffic related aerosol. These m/z's are mainly hydrocarbon ion fragments ($C_4H_7^+$ and $C_4H_9^+$) and are typically seen in a mass spectra of vehicle exhaust. Additionally, the multi-linear engine (ME-2) are used for source apportionment of OA.

At both sites, NRPM1 was dominated by organic aerosol. At the urban background site, traffic-related OA had larger contribution to total OA in wintertime as highest f55 and f57 values were detected on December and lowest during warmer months (Aug-Sep, 2016 and April-May, 2017). At the street canyon site, no clear seasonal patterns were observed, although the highest values of f55 and f57 were observed on December. Regarding the diurnal variation, f57 had more pronounced diurnal variation at the curbside than at the urban background while f55 was similar during the day at both sites without any clear diurnal variation.

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10SA.28

Regional Air Pollution Transport and Its Influence to Pollution Hot Spot in the Czech Republic. Jana Kozáková, Petr Vodička, Petra Pokorná, Lucie Ondráčková, Jakub Ondrácek, Jan Hovorka, Kamil Křůmal, Pavel Mikuška, Pavel Moravec, JAROSLAV SCHWARZ, *Institute of Chemical Process Fundamentals of the CAS, v.v.i*

The Upper Silesia includes a large area with a high concentration of industry and very poor air quality. The dominant part of the industrial area is located in the Polish Silesian province and a small part in the Czech Moravian-Silesian Region, where one of the European air pollution hot spots is the Ostrava city. Increased levels of air pollution have been associated with cardiovascular and respiratory diseases and other health consequences in adults and children.

The aim of the study was to elucidate the influence of local and regional air pollution sources on air quality in Ostrava Radvanice. This site is influenced by an air pollution from a local metallurgy complex situated in southwest (SW) direction. In addition, a regional pollution transported from the Polish Silesian Province (northeast-NE direction) can influence the whole Ostrava city.

In order to achieve this, a measuring campaign was carried out at the urban site of Ostrava Radvanice and in a suburban locality of Ostrava Plesná in the winter from 6th Feb 2014 to 6th Mar 2014. At both sites PM10 and PM1 mass concentrations were determined every 24 hours and mass size distribution of atmospheric aerosol was measured by cascade impactors every other day. Chemical analyzes of PM10, PM1, and impactor samples were performed. The meteorological parameters from the nearest weather monitoring stations were used to determine the relationship between the level of air pollution and the meteorological situation. A Positive Matrix Factorization (PMF) was applied to the 24h data set to apportion the sources at both sites.

Higher average mass concentrations of PM and chemical species were measured in Radvanice than in Plesná, with the exception of nitrate, sulfate, and ammonium ions in both PM fractions. Sodium and calcium ions in PM1 were four times higher and calcium and magnesium ions in PM10 even five times higher in Radvanice than in Plesná.

To investigate the influence of the metallurgy complex in Radvanice, the ratios between the mass concentrations measured in Plesná and Radvanice during SW and NE wind directions (WD) were calculated. During SW WD, the mass concentration in Radvanice was significantly higher than in Plesná, and therefore the influence of the metallurgy complex in Radvanice was evident. This finding was also confirmed by the increased mass concentrations of chemical species that are specific for this type of industrial sources. The influence of the regional air pollution was evident at both sites during NE WD, when the mass concentrations of PM and chemical species were increased. PMF revealed six and five sources for the PM10 and PM1, respectively, at both sites.

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10SA.29

Analysis of Particulate Atmospheric Matter Samples Collected with High Time Resolution: Some Examples of Recent Applications. FRANCO LUCARELLI, Giulia Calzolai, Massimo Chiari, Silvia Nava, Roy M. Harrison, Zongbo Shi, Di Liu, Bill Bloss, Van Tuan Vu, *University of Florence and INFN Florence, Italy*

The study of atmospheric particulate matter (PM) is an important issue, due both to the danger it poses to health and to its role in climate changes: these effects are strictly dependent on the chemical composition and the particle size. Most air quality studies on particulate matter (PM) are based on 24-h averaged data; however, many PM emissions as well as their atmospheric transport and dilution change within a few hours and daily samples are not capable of tracking these rapid changes. Elemental concentration obtained with 1-h time resolution can give invaluable information for the study of episodic events, lasting a few hours which may lead to an exposure problem like the ones occurring in industrial sites or during pyrotechnic events, such as on New Year's Eve, national festivities, and light festivals. Source apportionment receptor models need a series of samples containing material from the same set of sources in differing proportions and increasing the time resolution of the measurements typically provides samples that have greater between-sample variability in the source contributions than samples integrated over longer time periods. Furthermore, a more direct correlation with wind direction and speed is possible, since on a daily scale the wind direction may have strong variations. Finally, the choice of the sampling sites, along the prevalent wind direction and in opposite position with respect e.g. an industrial site, allows to follow the impact of the plume as a function of wind direction.

Currently, there are only a few devices available on the market for sampling aerosol with hourly resolution. At LABEC laboratory at Florence (Italy) since many years we use the so called "streaker" samplers by PIXE International Corporation, which are designed to separate the fine (<2.5 µm) and the coarse (2.5–10 µm) fractions of PM. These samples are effectively analyzed in a short time by PIXE technique at the LABEC laboratory, equipped with a 3MV particle accelerator, thanks to an optimized external-beam set-up, a convenient choice of the beam energy and the choice of suitable collecting substrata.

Examples of recent application of the combined use of streaker samplers and PIXE analysis (eventually complemented by other hourly data) will be reported, regarding industrial sites, heavy polluted towns (like Beijing or Delhi) or natural events (like Saharan dust transport episodes).

10SA.30

Contribution of Primary and Secondary Particles to Mode-Segregated Aerosol Particle Number Concentrations in Four European Cities. IOAR RIVAS, Cristina Reche, David Beddows, David Green, Leena Järvi, Christoph Hueglin, Hilkka Timonen, Gary W. Fuller, Jarkko Niemi, Markku Kulmala, Roy M. Harrison, Andrés Alastuey, Xavier Querol, Frank J. Kelly, *King's College London*

Atmospheric ultrafine particles may have a primary (directly-emitted) or secondary origin (formed from gas-phase precursor compounds). Primary particle number concentrations are estimated by applying an empirical scaling factor to Black Carbon (BC) concentrations (Rodríguez and Cuevas, 2007). The factor corresponds to the slope of the lower edge of the correlation between BC and particle number concentration (N) at morning traffic rush hours. As the relative contribution of primary and secondary particles may vary by region and time, we investigated these contributions during 2009-2016 at urban background stations (UB) in four European cities: Barcelona, Helsinki, London, and Zurich. These cities are characterized by different climatic and emission patterns. Moreover, a street canyon site in Helsinki was also assessed during 2015-2016. We investigated separately the contribution to total (N, measured with a Condensation Particle Counter), nucleation (Nnuc, particles <25 nm), Aitken (Nait, 25-100 nm), and accumulation (Nacc, 100-500 nm) modes (from a Differential/Scanning Mobility Particle Sizer). The size ranges for N and Nnuc varies due to different instrumentation used. Total N includes particles from 5 nm to 1 µm (N_{5-1000}) in Barcelona, $N_{10-1000}$ in Helsinki, N_{7-1000} in London, and N_{4-3000} in Zurich.

Zurich and Barcelona registered the highest N (13000 cm^{-3} and 12500 cm^{-3}, respectively) among the UB stations, followed by London (10500 cm^{-3}) and Helsinki (5200 cm^{-3}). Concentrations at the traffic site in Helsinki were higher than any of the UB (13700 cm^{-3}). Regarding BC concentrations, London (1.45 µg m^{-3}), Barcelona (1.28 µg m^{-3}), and the traffic site in Helsinki (1.25 µg m$^{-3)}$ registered the highest levels, being much lower in Zurich (0.87 µg m^{-3}) and Helsinki UB (0.39 µg m^{-3}).

Preliminary results suggest similar primary and secondary relative contributions at all studied UB stations. For all modes, the contribution of secondary particles was higher than the contribution of primary particles. On average for all cities and modes, particles from secondary origin was estimated to be 57%. The highest secondary contribution was observed in the nucleation mode at all cities, except at Zurich where it was in the Aitken mode. Generally, higher secondary contributions were observed during the spring and summer months, when higher solar radiation and temperatures took place. This is particularly important in Barcelona when secondary contributions to N are on average of 80% during midday summertime due to photochemical nucleation processes.

When comparing the urban background and traffic site in Helsinki, a slightly higher contribution of primary particles to total N were observed in the traffic site. When looking at the different modes, primary contribution at the traffic site is particularly higher at the Aitken and accumulation modes when compared to the urban background site. Traffic sites in urban areas influenced by diesel vehicles emissions have reported a mode around 30-40 nm for ambient air ultrafine particles size distributions (Dall'Osto et al., 2012), which would mainly affect the Nait.

Positive Matrix Factorization (PMF) applied to particle number size distributions is an effective method to assess the sources contributing significantly to N. The next step is to combine and compare the results from both methods allowing us for a better estimation and understanding of the contribution of primary and secondary particles to number concentrations.

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10SA.31

Advanced Receptor Models as a Tool to Improve the Knowledge of Aerosol Emission Sources at a Hot-Spot Pollution Site (Milan – Italy). ROBERTA VECCHI, Vera Bernardoni, Alessandro Bigi, Giulia Calzolai, Miriam Elser, Paola Fermo, Alice Forello, Franco Lucarelli, Dario Massabò, Silvia Nava, Andrea Piazzalunga, Rosaria Erika Pileci, Paolo Prati, Sara Valentini, Gianluigi Valli, *University of Milan & INFN-Milan (Italy)*

Emission sources and processes in atmosphere affect size distribution and chemical composition of atmospheric aerosol which are the main parameters responsible for aerosol effects at both local and global scale. Thus, understanding sources and processes leading to the measured concentrations in atmosphere is mandatory to develop suitable and effective abatement strategies.

Hot-spot pollution areas are peculiar sites where source emissions and meteorological conditions foster particulate matter accumulation, thus very high aerosol concentrations are often registered. The Po Valley (Northern Italy) – where Milan is located – is one of the main hot-spot pollution areas in Europe, especially during wintertime.

In this work, we present results from advanced receptor modelling approaches applied to aerosol collected with different sampling strategies in Milan (Italy) with the aim of improving the information generally obtained by traditional (e.g. Positive Matrix Factorization) receptor modelling.

The first example we will present is related to multi-time receptor modelling (Zhou et al., 2004), which allows a source apportionment study using all data with their own time resolution. This exploits the potentialities of high-time resolved measurements – e.g. allowing to detect sources acting for short periods – at the same time providing for such sources profile information also for components which are not measured with high time resolution.

To this aim, 1-h resolved elemental composition was measured by Particle-Induced X-Ray emission and 4-wavelength light absorption coefficient was determined by the polar photometer PP_UniMI (Bernardoni et al., 2017). In parallel, 24-h (during summer) or 12-h (during winter) resolved data of mass concentration, elements by Energy-Dispersive X-Ray Fluorescence, inorganic ions by ion chromatography, organic and elemental carbon by thermal-optical transmittance method, and levoglucosan by high-performance liquid chromatography coupled to pulsed amperometric detection were determined on 47 mm PTFE (for elements) and quartz fibre filters (for other components).

Another example of advanced source apportionment is the 3-way source apportionment (Ulbrich et al., 2012). In particular, a vector-matrix model (Tucker 1 model) was implemented. In this model, each element of the 3-D input matrix (representing the M species of the aerosol collected in N stages of a cascade impactor during R samplings) is factorised in S (unknown) factors. As reported in Bernardoni et al. (2017b) the model (implemented with Multilinear Engine 2, ME-2) was applied to size segregated aerosol samples collected using a Dekati-SDI cascade impactor (12 stages in the range 45nm-8.5µm) at an urban background station in Milan, Italy, during a winter period. Fourteen samplings were carried out with the cascade impactor, for a total of 168 samples available. All samples were collected on polycarbonate membranes. Elemental composition (Si-Pb) was determined by Energy-Dispersive X-Ray Fluorescence, the main inorganic ions (nitrate, sulphate and ammonium) by ion chromatography (IC), and levoglucosan (marker for wood burning) by high-performance liquid chromatography coupled to pulsed amperometric detection.

Special features of the results obtained with this model will be evidenced, such as the ability of identifying two sources related to traffic (i.e. diesel and gasoline), or the possibility to associate secondary compounds rapidly formed to specific sources (Bernardoni et al., 2017b).

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10TO.2

Partitioned Particulate Data and Health Risk Quantification of Metal Content in Mixed Residential Areas of Northern India. AJAY TANEJA, *DR. B.R.A. University, Agra, India*

The work presents the investigation of indoor air pollution through analysis of size segregated aerosol data (>2.5 µm, 2.5-1.0 µm, 1.0-0.5 µm, 0.5-0.25 µm) in varied residential homes separated by income and location at Agra, India. The study offered that discrepancy in lifestyle and indoor activities affects indoor particle mass concentration level dependent upon the source and house characteristics. Around 28-39% increased particulate concentrations were reported in low socio-economic homes than higher waged homes. A cascade impactor with PTFE filters collected particulate matter (PM) pollutant in coarse (>2.5 µm) and fine (quasi-accumulation ranges) (2.5-1.0, 1.0-0.5, 0.5-0.25 µm). Elevated loading for smaller size particulates (PM0.5-0.25= 54.08 µg/m3) was observed. Three main behavioural groups were identified following the size partitioning trend of elements (a) elements: Fe, Ca, Cr, Cu concentrated in coarser particles (b) elements distributed mainly within fine particle ranges: Zn, K, Al, Pb, Ni and (c) elements: Mn and Mg exhibiting indefinite partitioning pattern. Fine to coarse mass concentration ratio of all metals except Fe and Cr indicated their derivation from anthropogenic indoor sources. Enrichment factor and correlational analysis gave insight of the potential sources of metals. Bioavailability index further calculated showed the importance of smaller size particles in simulated lung environment that further varied with element (21% for Pb) and size (higher in PM0.5-0.25) elucidating increase in aerosol enrichment to finest particle. Higher non-carcinogenic and carcinogenic threats were embedded within Mn (HQ= 12.1) and Cr(VI) (ELCR= 1.21*10-3 (adults); 3.63*10-4 (child)) in fine (PM2.5-1.0) and coarser (PM>2.5) fractions respectively. Results of this work provide insight into size segregated particulate monitoring and address need for inclusive investigation to study its toxicity and control measures in establishing safer indoor environment.

10TO.3

Size-resolved Endotoxin and Toxicity of Ambient Particles in Beijing and Switzerland. YANG YUE, Haoxuan Chen, Ari Setyan, Miriam Elser, Maria Dietrich, Jing Li, Ting Zhang, Xiangyu Zhang, Yunhao Zheng, Jing Wang, Maosheng Yao, *Peking University*

PM2.5 pollution has become a global health concern, however its size-resolved toxicity remains to be poorly understood for different geophysical locations. Here, we have studied the size-resolved particulate matter (PM) mass, metal and endotoxin distributions as well as their related toxicity in two regions (Beijing and Switzerland) with stark difference of air quality. Ambient airborne PM samples were collected from selected sites into 13 different size ranges (10 nm - 18 µm) using a cascade multi-stage impactor (NanoMoudi).

The results showed that the two different regions had strongly different PM mass distribution patterns. For example, the Swiss urban samples had a peak size at 40 nm with 23.3% of the total PM mass, while the Beijing sample featured two peak sizes at 0.75 µm and 4.23 µm with 13.8 - 18.6% and 13.7% - 20.4% of the total PM mass, respectively.

The oxidative potentials were analyzed by the dithiothreitol (DDT) assay, and the results revealed that PM in different sizes had different oxidizing potentials. The PM oxidative potentials were also depended on the PM source, even within the same city, e,g, a campus and a farm. For Beijing, the particles with the highest oxidative potentials were detected at size ranges around 40 nm, 130 nm, 240 nm and 7.48 µm; while for Swiss urban, they are located in the size range of 0.01 – 1 µm.

Metal analysis results indicated that the Beijing samples had higher Cd, As and Pb in the size range of 0.1 – 1 µm, while the Swiss samples had higher Cu, Mn and Fe in the size range above 10 µm. Particularly, the Swiss urban samples had higher Cr levels at 1 µm.

Furthermore, the endotoxin results showed that different environments had different size-resolved endotoxin distributions, typically having one peak in the ultrafine size range (40-100 nm) and another in the larger size range (1.3-13.4 µm). More importantly, endotoxin activity was detected in the PM with size well below 1 µm, which can penetrate down to the alveoli and can be translocated into the cell tissue and/or circulation system.

These data suggest strong differences in the emission sources and particle formation mechanisms for different cities, thus resulting in different oxidizing potentials. Accordingly, use of only the PM mass concentration could lead to erroneous concussions regarding its health effects. Endotoxin distribution suggested that larger particles could also possess strong oxidation potential. The obtained information can facilitate optimization of the air pollution control strategies, while maximizing health and economic benefits.

10TO.4

Differential Toxicities of Airborne Fine Particulate Matter from Various Sources: A New Health Index for Monitoring Health Effects. MINHAN PARK, Hungsoo Joo, Kwangyul Lee, Myoseon Jang, Sang Don Kim, Injeong Kim, Lucille Joanna Borlaza, Heung-Bin Lim, Han-Jae Shin, Kyu Hyuck Chung, Yoon-Hyeong Choi, Sun Gu Park, Min-Suk Bae, Ji Yi Lee, Hangyul Song, Eunbi Lee, Enrique Cosep, Wajih Ur Rehman, Daeun Kim, Kihong Park, *GIST*

Fine particulate matter (PM) in the ambient atmosphere are strongly associated with adverse health effects. However, it is unlikely that all fine particles are equally toxic in view of their different sizes and chemical components. In this study, toxicity and chemical composition of PM produced from distinct sources (combustions sources (diesel engine, gasoline engine, biomass burning, and coal burning) and non-combustion sources (road dust, sea spray aerosols, ammonium sulfate, and ammonium nitrate)) including secondary organic aerosols produced from toluene, 1,3,5-trimethylbenzene (TMB), isoprene, and α-pinene under natural sunlight were evaluated. Multiple biological and chemical responses (oxidative potential, cell viability, genotoxicity (mutagenicity and DNA damage), oxidative stress, and inflammatory response) of various source-specific aerosols were integrated to derive source-specific toxicity and inhalation dose scores. Diesel engine exhaust particles were found to be the most toxic among the tested aerosols. A new health index was derived based on the differential toxicities and sizes of local and regional $PM_{2.5}$ sources as well as ambient concentrations of $PM_{2.5}$, and this new health index was observed to be more strongly associated with COPD mortality than $PM_{2.5}$ mass. The new health index can be potentially served as a useful indicator to estimate the adverse health effects caused by different fine particle types and provide practical management of PM beyond what can be achieved using PM mass which is the current regulation standard.

10TO.5

Characteristics and Health Impacts of Particulate Matters Emitted from A Typical Container Ship. DI WU, Qing Li, Xiang Ding, Jianfeng Sun, JianMin Chen, *Fudan University*

Maritime transport is a globally important source of pollutant emissions. Container ships have been widely recognized as the largest contribution of pollutant emissions among the maritime transport. Heavy fuel oil (HFO) and diesel oil (DO) are the two most commonly used fuels in Chinese container ships. However, characteristics and health impacts of particulate matters (PMs) emitted from real-world typical Chinese container ships of burning various fuels have been less systematically investigated. Aiming to compare the effect of HFO and DO, this study reports experimental results of PMs sampled via conducting a field campaign in coastal area of Shanghai, China. Since Results of pollutant emissions and their health effects will be comparatively presented. PM2.5 emission factors of burning HFO and DO in the same vessel are about 3.15 and 0.92 g/kg fuel, respectively. 16 EPA polycyclic aromatic hydrocarbons (PAHs) contained in HFO and DO PM2.5 samples are about 9.2 and 2.0 mg/kg fuel, respectively. PM number size distributions both possess a bimodal structure with two peaks at ~22 nm and ~100 nm, while DO PMs are dominated by the ultrafine mode. Benzo[a]pyrene equivalent carcinogenic potency (BaPeq) has shown an increased tendency with smaller size for both HFO and DO size-segregated PMs. Reactive oxygen species activity and cytotoxicity of small-sized PM samples are both higher than that of large-sized ones. HFO PM2.5 samples are about 2.5 and 3.2 times higher than that of DO ones, while they are both much higher than that of atmospheric PM2.5 samples collected in Shanghai. The difference of health risks is possibly owing to PAHs and metal element contents. Comparing to DO, HFO combustion emits much higher amounts of known health-hazardous species (PAHs, transition metals). Thus, further regulation of the fuel quality is implicated to be an important approach for reducing PMs and health impacts from shipping emissions.

10TO.6

Impact of Vehicular Load on Toxicity Potential of Ambient Air by the Road-side in Northern Indian City. SHUBHAM RATHI, Anubha Goel, *Indian Institute of Technology Kanpur*

Toxicity potential, the ratio of the concentration of particle (nanoparticles) bound polycyclic aromatic hydrocarbon (PPAH) to the surface area of the particles has been suggested as a proxy for air quality. This technique was used to assess the influence of vehicle emissions on air quality by the roadside at two locations with different land use patterns and traffic density (one falls on the highway and other is a residential area) within Kanpur city, India in the year 2015. Regular monitoring of air quality and vehicle count was performed and data used to calculate toxicity potential and examine its relation to traffic flow. Both locations were found to have high toxicity potential (daily avg. >4 ng/mm^2) and values recorded varied diurnally with traffic density. It was surprising to note that highway location with higher vehicle density and more four-wheelers had less average toxicity potential (4.08 ng/mm^2) as compared to the site near the residential area (4.87 ng/mm^2) with the standard deviation of 1.61 and 3.53 respectively. This was primarily due to more number of two-wheelers in the residential area as compared to highway location. Petrol driven two-wheeler emit smaller size particles.

Through a questionnaire survey, a high correlation between registered and running vehicle in Kanpur was observed: 95 percent of vehicles running on-road are registered in the city itself among which majority are two-wheelers (71%). The primary objective of the questionnaire survey conducted at 30 different locations (petrol pumps and parking lot areas) of >3000 vehicles was to ascertain the percentage and nature of Kanpur registered the vehicle in whole traffic fleet. The last ten-year registered vehicle data from regional transport office (RTO) of Kanpur city was collected and trendlines for annually registered two-wheelers and the total number of vehicles was calculated. From the trendline, it was found that by the year 2020, registered two-wheelers are predicted to become 1.32 times of current number. The total vehicle count will also increase by 1.29 times during the same time.

With toxicity potential being already high for the year 2015 with the major contribution of 2Ws, and vehicle numbers to increase approximately 32% over the next few years, the impact on air quality and human health risk is likely to increase. Impact of mitigation strategies being promoted by government of India, like introduction of stricter emission norms BS – VI (similar to Euro VI), promotion of alternative fuel sources such as ethanol, which are known to have lower emissions, along with use of vehicles that are charged using solar power or electricity needs to be looked into more critically to ensure further worsening of air quality and resulting health risks are minimized.

Keyword: Toxicity potential, PPAH, vehicle growth, Prediction, Kanpur, mitigation strategy

10TO.7

Toxicity of Particles Generated from a Consumer Fused Deposition Modeling 3d Printer Using Animal, Cellular and Acellular Models. QIAN ZHANG, Michal Pardo, Jenny P.S. Wong, Aika Davis, Marilyn Black, Yinon Rudich, Rodney J. Weber, *Georgia Institute of Technology*

Studies have shown that fused deposition modeling (FDM) 3D printers designed for general public use emit high levels of ultrafine and fine particles. The potential toxicity of these particles was assessed through preliminary tests involving in vivo, in vitro cellular and acellular methods for particles generated by three different printer filaments. All methods showed toxic-related responses. Mice intratracheal exposure for 24 h showed inflammatory response as an increase of total cell count and influx of neutrophils in BALF. In vitro cellular assays showed a decrease in cell survival rates for both rat macrophages and human epithelial cells after 24 h exposure. 3D printer particles may produce oxidative stress responses as intracellular ROS generation was measured for both rat macrophages and human epithelial cells after 6 h exposures and the acelluar dithiothreitol (DTT) assay showed measurable levels of oxidative potential. There was consistency among the different tests. Particles generated from polylactic acid (PLA) filaments elicited similar levels of response as particles generated from acrylonitrile butadiene styrene (ABS) filaments, despite much lower exposure concentrations of PLA. Although further testing is needed, the results suggest exposures to FDM 3D printer particle emissions should be minimized.

10TO.8

In Vivo Toxicity of Soot Can Be Predicted from Both Surface Area Dose and in Vitro Assays. OTMAR SCHMID, Tobias Stoeger, *Helmholtz Zentrum Munchen, Comprehensive Pneumology Center*

Inhalation of insoluble particles is believed to cause an oxidative cellular stress response, which may lead to pulmonary or even systemic inflammation. In addition to concern about urban dust and particularly soot particles, an increasing number of engineered nanoparticles is expected to be emitted into the atmosphere due to the economic success of nanotechnology. In the interest of consumer and workers' safety fast, reliable and affordable screening techniques for (nano-)particle toxicity are required. In addition, animal protection demands the development of straightforward in vitro tests, which are verified against in vivo results. Responding to these demands we combined data on acute pulmonary inflammation in mice (in vivo) with a cell-free oxidative potency (in vitro) for six types of soot particles.

For soot particle, inflammatory responses are likely to be induced by serval pathways including oxidative potency of the soot core and detoxification of organic compounds (e.g. PAHs) (Stoeger et al., 2009). Following this hypothesis we correlated our data on acute pulmonary inflammation in BALB/cJ mice (influx of polymorphonuclear neutrophils (PMNs) into the lungs) 24h after intratracheal instillation of various doses of six types of soot particles with corresponding (in vitro) data from a cell-free oxidative potency assay (consumption of ascorbate (antioxidant) and expression of the cytochrome (CYP) P450 gene (Cyp1a1) gene in a murine epithelial cell line (LA4) as marker of the detoxification pathway.

With this approach more than 90% of the observed variation in in vivo inflammatory efficacy of soot could be explained by an additive linear model involving oxidative potency and Cyp1a1 expression. This is particularly remarkable, since the six types of soot used here represent a wide dynamic range of some of the most relevant physico-chemical properties, namely (primary) particle diameter (10-50nm), organic mass content (OC; 1-20%) and BET surface area (43-800m^2/g) (Stoeger et al., 2009; Matuschek et al., 2007). Consistent with our pathway hypothesis, oxidative potency contributed most significantly to low OC soot the toxicity of high O soot was dominated by the detoxification pathway (Cyp1a1 induction).

May be even more remarkably, BET surface area dose explained more than 90% of the observed variability of the in vivo inflammatory response. Moreover, the six types of soot particles investigated here show similar toxicity as many engineered nanomaterials such as TiO_2, amorphous silica or even many types of multi-walled carbon nanotubes (graphene sheets), if – and only if – the inflammatory dose-response is expressed in terms of surface area as dose metric (not in terms of mass, volume or number).

In summary, while the assessment of soot-induced acute inflammation in mice is well correlated to lung-deposited surface area dose, more detailed information on the involved pathways of toxicity and their relative contributions to in vivo toxicity can be deciphered by the employment of suitable in vitro assays. The soot particles investigated here do not show enhanced toxicity as compared other low-solubility, low toxicity materials. However, a wider array of soot particles should be investigated to further assess this issue.

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10TO.9

Novel Atmospheric Sampling Method for Determination of 10 Carbonyls in Electronic Cigarette Aerosols Using LC-MS/MS. PHILIP KUEHL, Yongquan Lai, Larry Mallis, Jacob McDonald, Yue Zhou, Steven Belinsky, *Lovelace Biomedical, 2425 Ridgecrest Dr. SE, Albuquerque, NM*

Introduction: The collection and analysis of carbonyls within aerosol sampling has long been performed by sample atmospheres on the sorbent tubing or in impinger solutions containing derivertization reagent of 2,4-Dinitrophenylhydrazine (DNPH), followed by external standard quantitation using derivertized carbonyls as references. These methods generally require a fair amount of labor have a scientific issue with the external standard quantitation methods in that the unknown samples and references were not analyzed in the same conditions, which may cause the inaccurate results. These issues have been highlighted in the sampling of electronic cigarettes (e.cigarettes). Electronic cigarettes (E-cigarettes) have received increasing health concerns because evidence has accumulated showing the presence of harmful chemicals, including carbonyls, in the e-cigarette aerosols. Therefore a novel method for collection and analysis has been developed.

Method: In this study, we proposed a new sample collection and preparation method where unknown samples and standards were derivertized in the same conditions, followed by sensitive and sensitive LC-MS/MS analysis to improve the quantification accuracy of electronic cigarette carbonyls. For the e.cigarette sample collection, one puff of E-cigarette aerosol samples was collected in 55 mL of syringe and 10 mL of the collected aerosol samples was then transferred to a 30 mL sealed vial containing 1 mL of acetonitrile solutions. Carbonyls were trapped in acetonitrile solution by rotating the trapping vials for 2 hours. The trapped carbonyl samples and standard carbonyl solutions were derivertized with DNPH at 37 ºC for 2 hours before adding stopping solution containing internal standard. The processed samples and standards were finally analyzed using LC-MS/MS method.

Preliminary Data: The developed method resulted in a linear range from 2.00 to 1000 ng/mL for acrolein, crotonaldehyde, diacetyl, propanal, butanal and pentanal, linear range of 10.0 to 1000 ng/mL for acetaldehyde, linear range from range from 50.0 to 1000 ng/mL for acetone, and linear range from 50.0 to 5000 ng/mL for formaldehyde. The developed method was applied to determine the carbonyls in E-cigarette aerosols. Interestingly, we discovered that there is a high correlation between the level of carbonyls and the number of corresponding puffs in the samples. For example, formaldehyde level was found at almost 40 folds higher in puff No. 11 sample, compared to that in puff No. 4 sample. We hypothesized that the temperature generated in the E-cigarettes increased with increasing puff number, which resulted in corresponding dramatic increase in carbonyl levels.

Novel Aspect: Simultaneously determine 10 carbonyls in E-cigarette aerosols

10TO.10

Reducing Toxicity of Welding Fume Particles by Amorphous Silica Encapsulation. RYAN WARD, Trevor Tilly, Sarah Robinson, Arantzazu Eiguren Fernandez, Tara Sabo-Attwood, Chang Yu Wu, *University of Florida*

Despite the current safety protocols involved in arc welding, the production of toxic metal fumes as byproducts poses serious health risks to industry workers. According to the Bureau of Labor Statics in 2013, over 575,000 individuals in the United States are involved in the welding industry and of that amount, 31% had experienced metal fume fever at least once in their career. This condition stems from the nanoparticles released by the fumes associated with the welding process and the subsequent reactive metal exposure to the respiratory system of workers, where chronic exposure can be detrimental to human health. The addition of tetramethylsilane (TMS) to the shielding gas of a welder has been shown to coat the surface of these particles in amorphous silica once generated, and because this silica is less toxic to human, the risk associated with inhalation of these fumes is significantly decreased. In previous studies this has been shown, though *E. coli* was used for toxicity analysis, which cannot be directly correlated to possible adverse health effects in humans. The method employed for toxicity analysis in this study, however, represents a novel procedure wherein human lung cell culture can be exposed immediately to nanoparticles. Welding fume particles were generated, diluted to different concentrations through an air dilution system, and measured by a Scanning Mobility Particle Sizer Spectrometer (SMPS) for their aerosol size distribution. Cell culture were then exposed to the diluted fumes through the DAVID (Dosimetric Aerosol in Vitro Inhalation Device) system, which condensed water vapor onto the welding fume particles to grow particle size and allow for efficient deposition of particles to cell culture at the air-liquid interface, where gaseous phase aerosol are deposited directly into liquid cell culture. This innovative system allowed for a real-time exposure of nanoparticles to cell culture vs. the classical use of filter collection and submerged exposure to liquid cell culture. Both TMS coated welding particles and non-coated particles were exposed to cell culture via this method and a toxicity analysis was performed through a lactate dehydrogenase (LDA) assay, which measured viability of cell cultures post-exposure. Optimization of a TMS infusion system has potential to significantly reduce the health impacts associated with the welding process. Additionally, this demonstrates the functionality of the DAVID system as an alternative to the conventional methods of cell culture exposure analysis that more closely resembles aerosol exchange in that human respiratory system.

10WA.2

Investigation of the Feasibility of Workplace On-Site Ultrafine Particle Respiratory Deposition Measurement. YI CHEN, Wei-Chung Su, *University of Texas Health Science Center at Houston*

Workplace ultrafine particles (UFPs) are an essential occupational health concern. It is vitally important to investigate the deposition of UFP in the human respiratory tract in order to correctly estimate UFP inhalation dosimetry for related workers. However, to date, UFP respiratory deposition experiments can only be conducted in laboratory settings using laboratory-regenerated UFPs which are considered not representative of the actual UFPs shown in the real workplace. As a result, the applications of these laboratory-based lung deposition data are limited. To improve the representativeness and application of the UFP lung deposition data as well as to overall advance the experimental method of UFP respiratory deposition study, this research developed an improved experimental approach to conduct UFP lung deposition experiments. The goal of this research is to enable on-site workplace UFP respiratory deposition measurement. The improved approach was designed by using two SMPS units, a human lower airway replica, and a series of modified airway replicas to directly estimate the UFP respiratory deposition fraction in each lung generation on the airway replica. The initial deposition data obtained from employing UFP surrogates showed that UFP lung deposition in individual lung generation can be efficiently and systematically measured. This result demonstrates the feasibility and the suitability of applying the improved experimental approach to workplaces with UFP exposure concerns for assessing worker's UFP inhalation dosimetry.

10WA.3

Release of Respirable Fibrous Dusts during Abrasive Machining and Fatigue Testing of Carbon-Fiber Composites.

DAPHNE BÄGER, Nico Dziurowitz, Judith Neuhoff, Barbara Simonow, Carmen Thim, Dominic Kehren, Daniela Wenzlaff, Asmus Meyer-Plath, Sabine Plitzko, *Federal Institute for Occupational Safety and Health (BAuA)*

Carbon fibers are distinguished by their combination of low material density, electrical and thermal conductivity as well as high tensile strength and Young's modulus. Their composites have found widespread application in high-performance or light-weight product components. Standard carbon fibers that generally exhibit a diameter of 5-10 µm are non-respirable and presumed to be uncritical in terms of inhalation toxicity. However, composite development and manufacturing involves abrasive machining and fatigue testing that may give rise to dust release. Here, we report the release aerosols containing respirable carbon fibers fragments from mechanical abrasion and failure of composites containing ultra-high modulus fibers.

Workplace emission measurements were conducted during mechanical processing and tensile fatigue testing of test specimen made of pitch-based carbon fiber composites. Aerosol release during mechanical abrasion of such composites was also studied systematically in laboratory tests using a zero particle background chamber performing grinding and milling under controlled conditions. Aerosols were characterized by means of condensation particle counts, aerosol spectrometry, lung-deposited surface area quantification as well as morphological classification and quantification of SEM images of track-etched membrane filters.

Different to previous studies on carbon fibers handling workplaces, our measurements revealed near-field concentrations up to 1,000,000 respirable fibrous objects of WHO fiber geometry per cubic meter. The observed asbestos-like morphology of the fragments together with the known high chemical inertness of graphitic carbon fibers, inducing long-term biopersistance, renders such types of aerosols very critical from the toxicological point-of-view.

In laboratory tests, strong differences in fracture mode were observed for polyacrylonitrile- and pitch-based carbon fibers. The ultra-high Young's modulus of pitch-based fibers is therefore assumed to induce the observed strong propensity to release respirable fibrous fragments due to intrinsic anisotropic structure orientation during the graphitization step. Such material structure-related fracture modes must be considered for occupational health and safety strategies.

The work emphasizes the importance of detailed SEM-based morphological characterization and classification of aerosols found in workplace atmospheres to reveal the presence of unexpected, process-related toxic dusts components that are not detectable even by contemporary online techniques.

10WA.4

Concentration Levels of Airborne Nanoparticles in Taconite Processing. NIMA AFSHAR-MOHAJER, Rebecca Foos, Karl Braun, John Volckens, Gurumurthy Ramachandran, *Johns Hopkins School of Public Health*

Most studies of health risks in taconite mining and processing have focused on respirable dust mass concentrations and elongated mineral particles. However, many ore processing steps generate large amounts of nano-sized aerosol. Such particles, particularly ultrafine particles (UFPs, those with an aerodynamic diameter smaller than 0.1 µm) have been linked to increased cardiovascular disease in urban air pollution studies. Ultrafine particles contribute very little to the overall mass but are abundant in number. There is some evidence that particle number and surface area concentrations may be better metrics of exposure than mass concentrations.

In this study, we monitored concentrations of the airborne nanoparticles at four major processing units of a taconite surface mine: crushing, dry milling, wet milling, and pelletizing (United Taconite Mine, Iron Junction, MN, USA). We used three stations of direct-reading instruments to estimate particulate mass concentrations (PM_1, $PM_{2.5}$, Respirable, and PM_{10}) and particulate number concentrations (PN) and lung-deposited surface area concentrations (LDSA) of the nanoparticles, on two different days. Results revealed that pelletizing operation produces the highest nano-aerosol pollution as measured by three Partector (Naneos GmbH, Windisch, Switzerland), three DiSCmini (Testo GmbH, Titisee-Neustadt, Germany) nano-aerosol monitors, and two DustTrak (Model 8534, TSI Inc., St. Paul, MN, USA), on both days. However, the maximum instant LDSA concentrations (323 µm^2/cm^3 as measured by Partector units and 409 µm^2/cm^3 as measured by DiSCmini units) were related to the crushing operation. In Day 1, the average concentrations of nanoparticles across processing operations, from the highest to the lowest, were: (LDSAPartector = 192 µm^2/cm^3, LDSADiSCmini = 144 µm^2/cm^3, PN = 1.55×105 #/cm^{3,} PM_1: 199 µg/m^3 in the pelletizing operation; LDSAPartector = 125 µm^2/cm^3, LDSADiSCmini = 142 µm^2/cm^3, PN = 1.54×105 #/cm^3, PM_1: 148 µg/m^3 in the crushing operation; LDSAPartector = 96 µm^2/cm^3, LDSADiSCmini = 73 µm^2/cm^3, PN = 9.96×104 #/cm^3, PM_1: 97 µg/m^3 in the dry milling operation; LDSAPartector = 85 µm^2/cm^3, LDSADiSCmini = 77 µm^2/cm^3, PN = 9.06×104 #/cm^3, PM_1: 103 µg/m^3 in the wet milling operation. Power spectrum analysis was conducted to identify periodicity in the concentrations resulting from processing operations. The intraclass correlation coefficient (ICC) was used to evaluate between-day measurements.

10WA.5

An Experiment on Energy Consumption in an Indoor Water Spray Humidification Type Cleanroom with One Fluid Nozzles. Su-Bin Park, Won-Il Song, KYUNG-HOON YOO, Ji-Seok Yang, Deog-Yong Song, Oh-Myoung Kwon, Jungho Hwang, *Korea Institute of Industrial Technology*

In recent large-scale semiconductor manufacturing cleanrooms, the air conditioning energy consumption required to maintain cleanroom environment represents 40~50 % of the total power consumption in the factory. Therefore, the assessment on energy consumption in the air conditioning system of the cleanroom factory is essential for reducing the air conditioning load for the cleanroom. In particular, the energy consumption required to humidify outdoor air in the winter season is generally known to be enormous. Recently, in order to overcome the high energy consumption nature of a steam generator in a conventional steam humidification type cleanroom, a water spray humidification method with water spray nozzles is often introduced into cleanroom indoors instead of the steam generator in the outdoor air conditioning system. In the present study, a twin cleanroom experiment with an outdoor air flow of 2,300 m^3/h was conducted to compare at the same time the electric power consumption structure in a steam humidification type cleanroom and an indoor water spray humidification type cleanroom with one fluid nozzles. Besides, a numerical calculation was carried out to evaluate the annual power consumption of the two types of cleanrooms. It can be concluded from the present study that the indoor water spray humidification type cleanroom is more energy-efficient than the steam humidification type cleanroom. Furthermore it was shown from the numerical results that the indoor water spray humidification type cleanroom reduced 27 % of the annual electric power consumption of the steam humidification type cleanroom.

10WA.6

An Experiment on Energy Consumption in a High-Tech Electronics Industry Cleanroom with Dual Free-Cooling Heat Source. Su-Bin Park, Won-Il Song, KYUNG-HOON YOO, Ji-Seok Yang, Deog-Yong Song, Jungho Hwang, *Korea Institute of Industrial Technology*

So far, energy conservation issue has been important in electronics industry due to the regulation of global warming gas emission prevention. Besides, in a cleanroom for semiconductor manufacturing, energy saving demand for cleanroom facility is getting stronger because of worldwide price competition of a semiconductor. In such an electronics industry cleanroom with huge internal heat generation, annual continuous cooling is necessary and subsequent energy consumption becomes enormous. Free cooling is very effective for the reduction of the energy consumption in the cleanroom facility in the winter and intermediate seasons. Therefore, in the present article, we describe the present cleanroom facility with respect to the system configuration and operation method of cooling heat source. Finally, experimental energy consumption results with and without free cooling are compared in a way to find out maximizing the energy saving effect of cooling heat source system with dual free cooling operation.

10WA.7

Link the Oxidation Level between Gaseous and Particulates Compounds: A Study on Nitrogen-enriched Stainless Steel Welding and Cutting. JUN WANG, Marcio Bezerra, Jhy-Charm Soo, Shizhen He, Jacob Bartels, *University of Oklahoma*

Welding is a metal fabrication process commonly seen in different industries. The process relies on using high-temperature arcs to melt metals and hence either join or cut workpieces. Workers dealing with welding and cutting are exposed to highly oxidized metal particles and other gaseous pollutants emitted during the welding process. The most toxic oxidized metal in welding fume is hexavalent chromium (Cr^{6+}) which is a carcinogen with very low permissible exposure level. Nitrogen (Ni) in the surrounding air can also be oxidized to nitrogen oxides (NO_X) and present a potential health hazard. Our previous study showed there was a relatively strong correlation between the oxidation of nitrogen and chromium, which can lead to a potential low-cost and fast solution to detect Cr^{6+} level in the workplace by ubiquitous NOx sensor. In addition, nitrogen-enriched welding which employs nitrogen in the alloy to enhance resistance to sensitization, provide solid solution hardening, raise yield strength compared to non-nitrogen-enriched stainless steel. Nitrogen-enriched welding is growing in the nuclear industry when building structural material for reactors, as well as in cryogenic and biomedical applications. However, the extra nitrogen in the alloy coupled with nitrogen in shielding gases and surrounding atmosphere will create additional emission of nitric oxide (NO), nitrogen dioxides (NO_2), and potentially nitrous oxide (N_2O). The objective of this study is to investigate emission of NO_X and Cr^{6+} from nitrogen-enriched welding and to speculate if there is any correlation between them. A conical American Welding Society (AWS) fume chamber and high-volume air sampling pumps were used to collect welding fume. Nitrogen-enriched stainless steel metal plates (316LN) were welded and cut using a pulsed metal inert gas welder and a plasma cutter, respectively. Cr^{6+} in the fume was analyzed using an ion chromatograph following NIOSH 7604 method. NO, NO_2, and ozone were monitored by a GrayWolf air quality monitor with a toxic gas probe in both real-time reading in ppm and integrated total emission. N_2O was measured through a passive dosimeter. The results showed plasma cutting generally created more NO, NO_2, and Cr^{6+} than welding. Nitrogen-enriched stainless steel welding and cutting did not emit significant more NOx comparing to regular stainless steel. The NO and NO_2 concentration only showed a slight increase while welding with nitrogen-contained shielding gas. N_2O was detected during welding for the first time when welding under certain conditions. NO_2 was proved to have the best correlation with Cr^{6+} level (r=0.81). The results show a potentially promising technique to quickly respond to overexpose to Cr^{6+} by deploying NO_2 sensors. However, more field studies are needed before this technique can be widely adopted.

10WA.8

Measurements of the Physicochemical Properties of Nanoparticles Produced via Thermal Plasma Spraying Processes in a Precision Machining Workplace. Spyridon Bezantakos, Apostolos Salmatonidis, Mar Viana, GEORGE BISKOS, *Université du Littoral Côte d' 'Opale, Dunkerque, France*

Ceramic NPs (i.e., ceramic particles having sizes smaller than 100 nm) have received significant attention due to their unique properties that make them useful for a number of applications in diverse fields, including enhancing or altering the surface properties of engineering metallic parts. Concerns are raised regarding their human health implications due to the potential risk associated with their handling, manufacturing and from treating or manufacturing processes of bulk materials using ceramic NPs. In this study, we conducted measurements for determining the physicochemical properties (e.g., number concentration, size, shape, hygroscopicity and mixing state) of airborne particles in a machine shop that uses thermal plasma spraying for processing metallic engineering parts. In addition, samples of airborne NPs produced via the thermal plasma processes were collected in order to study their toxicity. The measurements were conducted at the workers breathing zone (i.e., inside the plasma spraying booths) when the plasma spraying processes were operational and during times of no activity (e.g., during night hours). Our first findings show:

1) The number concentration of fine airborne particles at the workers breathing zone when the plasma processes were active was by more than 100 times higher than that of the background, reaching some million particles/cm^3. This significant increase in the number concentration of aerosols was caused by NPs produced via the plasma spraying processes.

2) The size of aerosols produced from the plasma spraying processes was residing in the ultrafine fraction, in contrast to the background aerosols whose size distributions were characterized mainly by accumulation mode particles.

3) NPs emitted directly from plasma spraying processes are hydrophobic.

4) NPs directly emitted from plasma spraying processes in the workers breathing zone are externally mixed with the background aerosols (i.e., a hydrophobic and a hygroscopic population of aerosols can be observed). The fraction of the hydrophobic aerosol population depends on the concentration of NPs produced via the plasma spraying process. For example the lowest fractions of hydrophobic aerosols were observed when the plasma spray was not operational. However, when the plasma spray was operational and the concentration of NPs that were produced was much higher than that of the background aerosol population, only the hydrophobic mode was observable.

5) Larger particles (i.e., having dry electrical mobility diameters >60 nm) of the NPs produced via plasma spraying processes exhibited an apparent shrinking (i.e., their measured size at elevated relative humidity conditions was lower than of that selected at dry conditions). This behavior can be explained if these NPs had an elongated shape at dry conditions, which changed to a more spherical one when they interacted with water vapor inside the instrument. Further analysis using transmission electron microscopy (TEM), will provide additional information regarding the shape of the NPs produced via these processes.

11AC.1

Fog Processing of Aerosols Studied using HR-ToF-AMS and a Size Resolved CCN Counter. JAMES SCHWAB, Jie Zhang, Joseph P. Marto, Sara Lance, Yele Sun, *University at Albany, SUNY*

The effect of foggy conditions and aqueous processing on the characteristics of secondary aerosol was studied at Pinnacle State Park (PSP), NY in Sep. 2017, using an Aerodyne High Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS) and collocated instruments. The five day time period was marked by high relative humidity (>95%) for the five nights in the study, and radiation fog at the site on four of these nights. While thermodynamic and chemical conditions were largely favorable for new particle formation and growth, we believe that high RH and fog inhibited the potential occurrence of such events. At the same time, the high RH and fog conditions led to interesting and novel chemical interactions and signatures in the AMS organics. Three kinds of organic aerosols are identified through Positive Matrix Factorization of the aerosol mass fragment spectra. In particular, a biogenic secondary organic aerosol factor (BSOA) was evident, and this factor has been previously identified as associated with the gas-phase transfer though the reaction of biogenic volatile organic precursors with NO_3. Different fog periods will be identified by association with different chemical markers, and the influence of these fog periods on the aerosol properties (aerosol composition, size distribution, hygroscopicity, etc.) will be presented and discussed.

11AC.2

Burst of Hydroxyl Radicals in Newly-Formed Cloud Drops. SUZANNE E. PAULSON, Xiaobi Kuang, Jie Rou Chen, David Gonzalez, Peter J. Gallimore, John Scott, *UCLA*

Photochemical reactions age ambient particles and contribute to cloud processing of inorganic sulfur and organics, changing their chemical composition and enhancing aerosol mass concentrations. We show that during the first few minutes following cloud drop formation, the material in aerosols produces a large burst of hydroxyl radicals, resulting in concentrations in the 0.1 – 5 micromolar OH within the first two minutes. This is more OH than taken up from the gas phase or produced in the next several tens of minutes if the droplets are in bright sunlight. At micromolar concentrations, OH is far above Henry's law equilibrium. However, even low concentrations of dissolved organics should consume the majority of the OH produced in this initial the burst. Oxidation of organics in cloud drops will be enhanced over that currently in models.

11AC.3

Chemical Characterization and Source Apportionment of PM2.5 Aerosols in the Capital City “New Delhi” of India. S.N. TRIPATHI, Deepika Bhattu, Navaneeth M. Thamban, Vipul Lalchandani, Suneeti Mishra, Purushottam Kumar, Shashi Tiwari, Nidhi Tripathi, L.K. Sahu, S.B. Tiwari, Rangu Venkata Satish, Neeraj Rastogi, Atul K. Srivastava, Deewan S. Bisht, Suresh Tiwari, R. Sutaria, M. Mohan, Dilip Ganguly, Sudipta Ghosh, Pawan Vats, A. Tobler, Varun Kumar, P. Rai, Veronika Pospisilova, Giulia Stefenelli, *IIT Kanpur*

New Delhi, an Indian megacity suffers from the intense pressure of urbanization, industrialization and densely populated regions. These potential factors have caused sequential degradation of ambient air quality (300% higher $PM_{2.5}$ than NAAQS) and have been estimated to cause ~12000 premature deaths per year [1]. In last five years (2010-2015), a rapid increase (10 ug m^{-3}) in the population-weighted $PM_{2.5}$ mean concentration over India has been observed and attributed to fifth-ranking mortality risk factor[2]. Additionally, high pollutants concentrations also lead to urban and regional haze, deleterious impact on the regional ecosystem, crop yield and climate change. Consequently, more ambitious and strict control strategies together with the financial incentive schemes are required to have speedy changes in $PM_{2.5}$ levels and life expectancy.

Despite of the past efforts (1996-2010)[3], such as, cutting down the sulfur content of diesel and petrol and transition (2002) to compressed natural gas (CNG), and shutdown of the “hazardous” industries, the annual average $PM_{2.5}$ levels persisted at alarming levels (110-120 µg m^{-3}) during 2011-2015. Recent attempt of $PM_{2.5}$ mitigation as “odd-even traffic intervention, 2016” policy was also proven with no success[1]. However, to understand the impact of such desperate policy measures and redesign the effective strategies, a more precise long-term characterization and source apportionment of organic/inorganic gaseous and particulate phase species at both local- and regional-scales is required.

Here, we combine a comprehensive set of novel and hybrid approach (offline and online) with statistical techniques to understand the sources and chemical nature of fine particulate matter (PM) in New Delhi. Ambient measurements are performed at 5 sites extending to both upwind (Hisar) and downwind (Kanpur) of New Delhi (IITM, IIT Delhi and MRIU). Sampling sites in New Delhi are partly surrounded by dense vegetation and affected by a mix of local traffic and residential activities. Real-time particle phase organic and inorganic composition at Delhi sites are measured by Aerodyne’s aerosol mass spectrometer (AMS) and time-of-flight aerosol chemical speciation monitor (ToF-ACSM), and extractive electrospray ionization long-time-of-flight mass spectrometer (EESI-LToF-MS), and organic gases using proton transfer reaction time-of-flight mass spectrometer (PTR-ToF-MS). Further, particle number concentration and size distribution (up to 20 µm) are obtained by integrating scanning mobility particle sizer (SMPS, TSI) and optical particle sizer (OPS, TSI) and/or aerodynamic particle sizer (APS, TSI). In addition, real-time BC mass concentration and size distribution, WSOC and BrC, and multi-metal concentrations are measured by 7-wavelength Aethalometer and single particle soot photometer (SP2), particle-into-liquid sampler coupled with a liquid waveguide capillary cell and total organic carbon analyzer (PILS-LWCC-TOC) and XACT®625i, respectively. Supporting meteorological parameters (wind speed, wind direction, RH, Temp. and precipitation) and gas concentrations are provided by automatic weather station (AWS), and O_3, SO_2, CO and NO_x analyzers. Concurrently, day and night time $PM_{2.5}$ filters collected from all 5 sites are further analyzed for (a) WSOC content by newly developed mass spectrometric techniques, (b) EC-OC content, (c) radiocarbon (^{14}C), (d) ions and (e) trace metals. Further, to understand space-time variability, hot spots and contribution from local vs regional sources and validate satellite observations and chemical transport models, a network of 25 low cost optical aerosol sensors ($PM_{2.5}$ and PM_{10}) over square grids in National Capital Region of Delhi have also been deployed.

The results of this study will aid in linking the sources and day and night atmospheric processing of the emissions, further elucidating the production pathways of secondary organic aerosol and health relevant oxygenated species. It will provide the relevant information to the regulatory authorities concerning abatement technologies to reduce the environmental, economic and health impacts resulting from particulate pollution.

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11AC.4

Observed Below-cloud Aerosol Chemical and Physical Properties on Whiteface Mountain, New York during August 2017. JIE ZHANG, Sara Lance, Richard Brandt, Joseph P. Marto, Matthew Ninneman, James Schwab, *University at Albany, SUNY*

A pilot study took place at Whiteface Mountain (WFM) in the Adirondacks of upstate NY during the summer of 2017 to study the chemical processing of organics within clouds. The below-cloud submicron aerosols were characterized in real-time from onboard the ASRC Sprinter van using an Aerodyne High Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-TOF-AMS), a TSI Scanning Mobility Particle Sizer Spectrometer (SMPS), a DMT Cloud Condensation Nuclei counter (CCNc), and a TSI Condensation Particle Counter (CPC). The HR-TOF-AMS measurements are used to analyze chemical composition of below-cloud aerosols focusing on different organic factors, which are then compared with offline HR-TOF-AMS measurements of bulk cloud water samples collected at the summit during the same time period. Aerosol size distribution and CCN activation efficiency measurements at the summit are compared to the below-cloud measurements as well (using the same instruments). Differences in the measurements under clear and cloudy conditions are explored to probe the potential influence of aqueous chemical reactions on secondary organic aerosol formation.

11AC.5

Formation of Secondary Organic Aerosol (SOA) during Winter in the Eastern United States. MARWA EL-SAYED, Christopher Hennigan, *University of Maryland, Baltimore County*

The aim of this study is to characterize the formation of secondary organic aerosol (SOA) during the winter in Baltimore, MD through simultaneous measurements of water-soluble organic carbon in the gas ($WSOC_g$) and particle ($WSOC_p$) phases. Two main processes were responsible for the wintertime SOA formation, namely: (1) gas-phase and (2) aqueous processes (aqSOA). SOA formation through the gaseous phase was interpreted based on the relationship between the partitioning coefficient, $F_p = WSOC_p/(WSOC_g + WSOC_p)$, and organic carbon (OC) concentrations. An increase in F_p as a function of OC indicates that the partitioning was dependent on the amount of pre-existing aerosol suggesting SOA formation through traditional gas-phase partitioning. Such a relationship was observed during colder periods, only (< 0 ^oC). At night, an enhancement in F_p was observed with increasing relative humidity (RH) for temperatures between 0 and 10 ^oC, suggesting the occurrence of aqSOA formation in aerosol liquid water (ALW) solely in this temperature range. For the periods < 0 ^oC and > 10 ^oC, there was no relationship between F_p and the RH, implying that aqSOA was not substantially formed under such conditions. A climatology of ALW during the winter showed a striking temperature dependence, with low ALW levels when the temperature was below 0 ^oC. Using back trajectories, we show that this observation was likely due to air masses from Canada/arctic associated with the lowest winter temperatures. Aerosol potassium concentrations were inversely correlated with temperature during winter, implying their link to biomass burning due to residential heating. Conditions for aqSOA formation occur in the winter when both ALW and sufficient biomass burning emissions are present – this corresponds to wintertime temperature between 0 and 10 ^oC in Baltimore. The $WSOC_p$ measurement was alternated between ambient ($WSOC_p$) and dry ($WSOC_{p,dry}$) channels to directly probe the effect of ALW evaporation on the SOA. A comparison of the $WSOC_p$ and $WSOC_{p,dry}$ concentrations indicated a $WSOC_{p,dry}/WSOC_p$ ratio of unity for the data in the range 0 – 10 ^oC, the conditions corresponding to aqSOA formation. This denotes that $WSOC_g$ compounds taken up in aerosol water, causing the enhancement in F_p, remained in the condensed phase upon drying due to their formation irreversibly. In addition, the $WSOC_{p,dry}/WSOC_p$ ratios were nearly constant across the entire RH range supporting the irreversible formation of aqSOA in the winter.

11AC.7

Simulating Secondary Organic Aerosol Formation in Cloudwater and Aerosols Using GAMMA 5.1. WILLIAM TSUI, Joseph Woo, V. Faye McNeill, *Columbia University*

Aqueous phase chemistry in cloudwater and aerosols is a known pathway of secondary organic aerosol (SOA) formation, yet its contribution in ambient conditions remains largely uncertain. In this study, we use Gas-Aerosol Model for Mechanism Analysis (GAMMA) version 5.1 to simulate SOA formation in particles alternating from aqueous aerosol to cloudwater. In acidic aerosols under low-NO_x conditions, formation of tetrol and organosulfate products from isoprene epoxydiols (IEPOX) is a dominant process. However, when these acidic aerosols convert to cloudwater, the extent of this SOA formation pathway was seen to reduce significantly due to a decrease in aqueous H^+ activity. Furthermore, particles initially in aerosol conditions for at least one hour were not observed to have organic acid formation upon transitioning to cloudwater. The lack of organic acid SOA is primarily due to the consumption of OH radicals in the formation of IEPOX under aerosol conditions, resulting in a depletion of radicals necessary for the generation of organic acids in cloudwater. Under high-NO_x conditions, cloudwater concentrations were found to be less dependent on the amount of time as an aerosol in the beginning of the simulation than low-NO_x conditions. Similar simulations of alternating cloudwater and aqueous aerosols are conducted using gas-phase concentrations from Whiteface Mountain as initial conditions.

11AC.8

Direct Observations of the Formation of Isoprene-derived Secondary Organic Aerosol in Ambient Cloud Droplets. ALLA ZELENYUK, David Bell, ManishKumar Shrivastava, Jerome Fast, Joel A. Thornton, Dan Imre, Kaitlyn J. Suski, Larry Berg, John Shilling, Jiumeng Liu, Fan Mei, Jason Tomlinson, Jian Wang, *Pacific Northwest National Laboratory*

Multiphase chemistry of isoprene photooxidation products has been shown to be a major source of secondary organic aerosol (SOA) in the atmosphere, yet many models apply simplified treatments of organic aqueous chemistry. A number of recent studies indicate that aqueous aerosol phase provides a medium for reactive uptake of isoprene photooxidation products, and in particular, isomeric isoprene epoxydiols (IEPOX). Studies have shown that the reaction rates and yields of IEPOX-SOA formation depend on aerosol acidity, water content, sulfate concentration, and the presence of other organics. However, very few studies focused on chemistry occurring within actual cloud droplets.

We will present data acquired during recent ARM Holistic Interactions of Shallow Clouds, Aerosols, and Land Ecosystems (HI-SCALE) Campaign, which provide direct evidence for IEPOX-SOA formation in cloud droplets. Single particle mass spectrometer, miniSPLAT, and a high-resolution, time-of-flight aerosol mass spectrometer were used to characterize the composition of aerosol particles and cloud droplet residuals, while a high-resolution, time-of-flight chemical ionization mass spectrometer (HR-ToF-CIMS) was used to characterize gas-phase compounds, including isoprene and IEPOX.

We find that the size and composition of cloud droplet residuals were markedly different than those of aerosol particles sampled outside the cloud. Cloud droplet residuals were larger than particles outside the cloud and comprised of individual particles with high relative fractions of sulfate and nitrate and significant fraction of particles with mass spectra that are nearly identical to those of laboratory-generated IEPOX-SOA particles. Moreover, we show that the observed cloud-induced formation of IEPOX-SOA particles was accompanied by simultaneous decrease in measured concentrations of IEPOX and other gas-phase isoprene photooxidation products.

Finally, we use these HI-SCALE field observations of cloud residuals, interstitial aerosol particles, and gas-phase species to develop and evaluate model treatment of aqueous-phase isoprene SOA formation. We show that the addition of aqueous cloud chemistry to WRF-Chem qualitatively reproduces the observed concentrations of biogenic volatile organic compounds and the impact of aqueous-phase chemistry on cloud-borne organic mass.

11AP.1

Single Scattering Albedo of Agglomerated Debris Particles and Homogeneous Spheres: A Comparison. HANS MOOSMULLER, Evgenij Zubko, *Desert Research Institute*

The aerosol single scattering albedo (SSA) is the dominant intensive particle parameter determining aerosol radiative forcing in the earth's atmosphere [1-3]. We build on previous work that used Mie theory to examine the behavior of SSA as a function of size parameter x and complex refractive index m for homogeneous spherical particles [4,5].

Here, we investigate the behavior of SSA as a function of size parameter x for agglomerated debris particles [6] that are a much more realistic model for atmospheric mineral dust particles than homogeneous spheres. We use discrete dipole approximation (DDA) calculations to obtain SSA as function of size parameter and imaginary part of the refractive index. These results are compared with Mie theory results for homogeneous spherical particles and we show that SSAs for agglomerated debris particles and homogeneous spheres converge in the small particle and geometric optics regimes if complex refractive indices are adjusted properly using effective medium theory [7]. However, in the intermediate transition regime there are substantial differences in the SSAs of these two types of particles that greatly affect their radiative forcing.

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11AP.2

Comparing Refractive Index Retrievals of Size- and Mass-Selected Particles to Full Distribution Measurements: A Metrology Perspective. JAMES RADNEY, Christopher Zangmeister, *National Institute of Standards and Technology*

Retrieving refractive indices from measured optical and size and/or mass data for both ambient and laboratory aerosols has found significant use in recent years. Here, we compare results for refractive indices retrieved from measurements of size- and mass-selected particles to those using the full distribution (i.e. measurements typically performed in the laboratory versus field, respectively) with particles of various morphologies and compositions: single component (ammonium sulfate and nigrosin), homogeneous mixtures of ammonium sulfate and nigrosin at multiple mixing ratios and core-shell particles at multiple mixing ratios of ammonium sulfate and black carbon. Extinction and absorption coefficients, aerosol size (electrical mobility), mass and number concentrations were measured using cavity ring-down and photoacoustic spectrometers, a differential mobility analyzer, an aerosol particle mass analyzer and a condensation particle counter, respectively. We find that the two methods compare reasonably well for single component aerosols (≈ 5 % and 25 % deviations in the real and imaginary refractive indices, respectively) with significantly larger deviations in the imaginary component for the homogeneous mixtures and core-shell particles (≈ 50 %). Notably, neither measurement (size/mass selected or full distribution) can quantitatively capture the size dependence of the absorption cross sections to better than 30 % for the homogeneous mixtures or core-shell particles. Last, we will discuss the benefits, limitations and sensitivities of each method relative to all the measured parameters (extinction, absorption, number concentration, size and effective density).

11AP.3

Modification of Aerosol Properties Due to Relative Humidity. DANIELLE EL HAJJ, Suzanne Crumeyrolle, Marie Choël, Isabelle Chiapello, *Université de Lille*

Aerosols play vital roles in energy balance and human health. They have direct interaction with solar and telluric radiation by scattering and absorbing solar radiation, leading to, respectively, a cooling or warming effect of the atmosphere. The last assessment report by the *Intergovernmental Panel on Climate Change* (IPCC), states that the uncertainty in the total radiative forcing is mainly dominated by the high uncertainty in the aerosol radiative forcing. This is mainly caused by the poorly understood and quantified aerosol effects. Indeed, high relative humidity (RH), promotes water uptake by atmospheric aerosol particles (Pilinis et al., 1989), which modifies their size, morphology and chemical composition and therefore their optical properties (Zieger et al., 2013).

In-situ measurements of aerosols properties (scattering and absorption coefficients, size distribution) are usually performed at dry conditions (RH<40%) to avoid RH - effects when quantifying and characterizing the main aerosol properties. However, aerosols are present in a humid atmosphere. This is especially important for the aerosol properties that strongly depend on RH. Knowing the physical, chemical and optical properties of the aerosol particles at ambient RH is thus crucial in order to improve the estimation of the aerosol direct radiative forcing (Zhao et al., 2006: Kuang et al., 2016b).

The aim of this work is to study the evolution of aerosols optical (scattering and absorption), physical (size) properties of aerosols at different RH. Our study is based on laboratory measurements at controlled humidity. Pure aerosols were generated, such as sodium chloride (NaCl), ammonium nitrate ($(NH_4)_2SO_4$), sodium nitrate ($NaNO_3$) and potassium chloride (KCl). Pure aerosols were then mixed together taking into account their molar fraction within the binary mixtures of above-mentioned compounds. The study was first conducted under dry conditions (~35% RH) to validate the instrumental set up. Measurements were performed at higher RH (from 40 up to 90%) using a nephelometer (AURORA 3000) and a particle counter (WELAS).

The magnitude of the scattering enhancement factor f(RH) that mainly depends on aerosol chemical composition and size, is calculated. Thus the exchange of water vapor that causes a change in size and refractive index (RI) of aerosol particles and therefore directly influences its optical properties is computed using a thermodynamic model (ISORROPIA II) and an empirical method. Zdanovskii–Stokes–Robinson (ZSR) approach is applied on aerosols mixtures and compared with the experimental measurement. The discrepancies found will be presented and will be used to better understand the influence of water uptake on the radiative forcing estimated by climate models.

11AP.4

Elastic and Inelastic Scattering of Laser-Trapped Particles: Optically Characterizing Trace Aerosols. PATRICIO PIEDRA, Aimable Kalume, Yong-Le Pan, Gorden Videen, *U.S. Army Research Laboratory*

Optical detection of chemical and/or biological agents is a significant challenge since these particles can be present in the atmosphere in trace amounts. Optical detection of these agents requires exquisite accuracy to isolate the optical signal of a few particles in a background of numerous air molecules, other aerosol particles, and atmospheric compounds. Single particle laser-trapping is a technique pioneered at the U.S. Army Research Laboratory that allows us to capture a particle in the air for a prolonged time and collect very detailed information of the particle's elastic (i.e., Rayleigh, Mie scattering) and inelastic (i.e., Raman and fluorescent scattering) optical signal. In this study, we measure elastic and inelastic light scattering signal of several laser-trapped aerosol particles. Our measurements are analyzed, and multi-dimensional statistical clustering techniques are applied to mathematically group particles by their optical similarities in both elastic and inelastic scattering parameters. These clustering techniques are expected to yield significant differences between distinct types of aerosol particles. In future work, we expect to apply deep learning techniques to identify trace amounts of aerosols using data collected in our experiments. If this preliminary proof of concept is successful, it has the potential to lead to innovative studies aiming to improve remote sensing techniques of trace chemical and/or biological agents.

11AP.5

A Novel Mie Theory Inversion Technique for Retrieving the Complex Refractive Index from Optical Measurements.

BENJAMIN SUMLIN, William Heinson, Rajan K. Chakrabarty, *Washington University in St. Louis*

Mie theory is a powerful tool that can accurately calculate the scattering and absorption behavior of a particle with any radial symmetry, such as spheres and long cylinders, and whose diameter is on the order of the wavelength of incident light. However, the complex refractive index $m=n+ik$ is often the unknown parameter in aerosol optics studies and is a vital parameter for climate modeling and satellite retrieval algorithms. Mie theory equations take m as an input, therefore recovering it from measurements presents an inverse problem which is confounded by the multidimensional parameter space the equations require. Typically, Mie theory inversions are often constrained to the particle size and real m, but the specific inverse problem of recovering complex m from experimental measurements is the focus of this work.

Since m cannot be measured directly, a method to determine the refractive index from experimental data is needed. We present a novel, visual method to determine m from optical measurements by identifying intersections of scattering and absorption contour maps in n-k space. Our method allows arbitrary curves to be treated geometrically and algebraically, eliminating the need to develop complicated analytic expressions for the contours. The minimum inputs are scattering, absorption, particle size, and wavelength, however, this can lead to an improperly constrained problem, with multiple valid values of refractive index that will reproduce the measured parameters. This can be fully constrained by measuring an additional independent parameter, such as the backscattering efficiency.

Our method is presented in the context of The Python Mie Scattering package, or PyMieScatt, which was developed to be a complete tool for both forward and inverse Mie theory calculations. This package is open-source, fully documented, and available to the community, allowing research groups to bypass the step of developing their own Mie theory software.

11AP.6

Towards Statistical Analysis of Aerosol Hygroscopic Properties Using Raman Lidar Measurements. FRANCISCO NAVAS-GUZMÁN, Giovanni Martucci, Maxime Hervo, Martine Collaud Coen, Bertrand Calpini, Valentin Simeonov, Alexander Haefele, *Federal Office of Meteorology and Climatology, MeteoSwiss*

The uncertainty in assessing total anthropogenic greenhouse gas and aerosol impacts on climate must be substantially reduced from its current level to allow meaningful predictions of future climate. This uncertainty is currently dominated by the aerosol component. Aerosol particles scatter and absorb radiation as well as change the microphysical properties of clouds. Evaluation of aerosol effects on climate must take into account high spatial and temporal variation of aerosol amounts and properties as well as the aerosol interactions with clouds and precipitation. During the last years a huge effort has been made in order to characterize vertically-resolved profiles of optical and microphysical properties for different kinds of particles. Raman lidars (light detection and ranging) have proven to be an essential tool to obtain profiles of these properties without modifying the environmental conditions. An important factor that can modify the role of aerosols in the global energy budget is the relative humidity (RH). Under high relative humidity conditions, aerosol particles size may increase due to water uptake (hygroscopic growth) altering their size distribution. Therefore, hygroscopic growth affects the direct scattering of radiation and especially the indirect effects, as the affinity of atmospheric aerosols for water vapour is highly related to their ability to act as cloud condensation nuclei (CCN). Thus, understanding aerosol hygroscopic growth is of high importance to quantify the influence of atmospheric aerosol in climate models.

Despite its importance, aerosol hygroscopic properties have not been properly characterized yet using remote sensing techniques (non-invasive method) and it is an open issue that needs to be addressed. The number of aerosol hygroscopic studies is modest and most of them were limited to few case studies during specific field campaigns. The major limitation of most of these studies is due to the lack of simultaneous observations of vertically resolved profiles of relative humidity and aerosol properties.

The Swiss RAman Lidar for Meteorological Observations (RALMO) can overcome these difficulties since it is able to provide continuous daytime and nighttime profiles of aerosol properties (backscatter and extinction) and relative humidity. RALMO is a state-of-art humidity, temperature and aerosol profiler capable to measure the rotational-vibrational Raman signals of nitrogen and water vapour (wavelengths of 386.7 and 407.5 nm, respectively) along with the pure rotational Raman (PRR) signal around the Rayleigh line at 355 nm. RALMO is operated at the aerological station of MeteoSwiss at Payerne (46º48' N, 6º56' E, 491 m asl) since beginning 2008 and provides one of the longest time-series of vertical profiles of humidity, temperature and aerosol properties in Europe. The presented study shows several case studies where the capability of this lidar system to detect vertically and temporally resolved aerosol hygroscopicity is proved. In addition, a methodology to exploit the 10-year data set and to produce a solid statistical analysis of aerosol hygroscopic properties is presented. The results show the potential of RALMO dataset for future statistical analysis of hygroscopic properties for a large variety of particles that reach our station (e.g. volcanic particles, Saharan dust, pollution, biomass burning aerosols, etc).

11AP.7

Chemical and Optical Properties of Volcanic Ashes: Laboratory Measurements and Remote Sensing Applications.

ALEXANDRE DEGUINE, Denis Petitprez, Lieven Clarisse, Hervé Herbin, *Université de Lille*

During a volcanic eruption, a huge amount of aerosols are emitted into the atmosphere which can be transported over long distances. By absorbing and scattering radiation, volcanic ashes influence strongly the Earth radiative budget. These particles may also affect human health and for some intense events may perturb or interrupt air traffic.

Aerosols can be detected by remote sensing using in particular from infrared spectrometers. These instruments record the extinction signal of a mixing gas and aerosols contribution. From these observations, the main objective is to estimate the chemical composition, the size and the number concentration of the particles. However, the retrieval of these parameters needs to use the appropriate complex refractive indices m, which are mainly unknown and are, up to now, one of the main sources of uncertainty for studying aerosols from infrared remote sensing instruments.

For this purpose, a new methodology has been applied in order to retrieve complex refractive indices in a large spectral range from the measurement of the extinction spectra of various sampling aerosols. Volcanic ashes powder was dispersed by a mechanical agitation in a flow of nitrogen (5 L min-1) within a glass container. Then the aerosol flow is directed through two spectrometers recording the extinction spectra from UV-visible (MAYA 2000 PRO, Ocean Optics 200 to 1100nm) to Infrared (Antaris IGS Analyser, Thermo Scientific 2,5 to 25 micrometers) and finally to an aerodynamic particle sizer (TSI APS 3321) to record the size distribution in the range 0.5-20 micrometers. A combination of experimental data, Kramers-Kroning relationship and optimal estimation method is used to determine both the real n and imaginary κ parts of the complex refractive index.

This methodology has been successfully applied for five volcanic ashes samples collected from Chile (Cordon Caulle, Chaiten, Calbuco) and Iceland (Grimsvötn, Eyjafjallajökull). Moreover, a chemical analysis has been performed for each sample using X-ray diffraction (XRD) to establish the link between chemical and optical properties of materials. These results are then use to retrieve volcanic aerosol parameters from IASI/MetOp satellite instruments.

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11AP.8

Single Airborne Particle Studies Using Optical Trapping and Manipulations: What We Have and What We Have Not.

CHUJI WANG, Zhiyong Gong, Gorden Videen, Yong-Le Pan, *Mississippi State University*

Single airborne particles can be levitated, trapped, and transported in air using light force under an appropriate arrangement. Most airborne particles are nontransparent, therefore both radiation pressure force and photophoretic force account for the status of motion of the particles, which is often further compounded by many other factors, such as drag force, air turbulence, particle properties as well their changes overtime. This nature makes the single airborne particle study a challenging yet attractive topic. When a single particle is under light illumination in air, their time-dependent physical and chemical properties reveal exact particle dynamics without surface interferences from other particles. We can examine a single particle layer-by-layer, its chemical phase separation, morphology, up-take and evaporation, photochemical processes, fluorescence, Raman, and light-scattering. We can even now look at chemical compositions point-by-point within a single particle. We can also explore light controlled single particle's motion, momentum transfer, particle sorting, and even potentially 3D display. Significant strides have been made to touch each of the aforementioned points to date, yet many more challenges in single particle studies using optical trapping and manipulations have not been addressed. These challenges also offer us an exciting opportunity to better understand airborne particles and allow us to envision new applications. This talk will discuss what we have and what we have not in single airborne particle studies using optical trapping and manipulations.

11BA.1

Environmental Factors Affecting Biological Aerosols in Houston, TX. JOSHUA SANTARPIA, Sean Kinahan, Don Collins, Yong-Le Pan, Aimable Kalume, Matthew Tezak, Gabriel Lucero, Steven Storch, Cathryn Reyna, Danielle Rivera, Kevin Crown, *Sandia National Laboratories*

During the summer months of 2015 and 2016 several weeks of field experiments were performed at a site in the W.G. Jones State Forest near Conroe, TX. These experiments examined changes to intentionally generated biological aerosol (Bacillus thuringiensis) when exposed to the ambient environment of this area, comparing particles fixed onto artificial spider webs and suspended in a gas and UV permeable chamber. Throughout these experiments, extensive measurements of environmental factors such as solar flux and organic and inorganic trace gas were recorded. In 2015, experiments consisted exclusively of daytime experiments, while in 2016 a mix of daytime and nighttime experiments were performed. These studies used multiple chambers to allow different environmental factors to be controlled to attempt to isolate key factors impacting the particles. For instance, in some cases one chamber would be exposed to sunlight and all ambient gas-phase species, while another chamber would be kept isolated from solar radiation with its intake filtered to remove ambient species. This would potentially allow bioaerosols generated at the same time to be exposed to different conditions during the same time period to investigate the role of sunlight and chemical aging separately. In addition, particle growth rates were measured using a co-injected mode of inorganic, sub-micron particles as an indicator of secondary growth processes activity in the chamber. Biological aerosols were measured and quantified in several ways throughout the studies. Measurements compared changes in aerodynamic size and particle fluorescence spectra, as well as viability and qPCR signature. Comparison of these data under different environmental conditions and between the two chambers led to several key findings. This study clearly indicates that biological aerosol trapped on spider webs aged at the same rate as free biological particles suspended in the rotating drum chamber. In addition, the exposure to high solar intensities in Houston led to high decay rates, which dominate the decay in viability observed during most daytime experiments. Correlation analysis between changes in biological aerosol measurements and trace species concentrations and particle growth rates indicate several potential chemical aging pathways that affect both the DNA and proteins.

11BA.2

H2O2 Modulates the Energetic Metabolism of the Cloud Microbiome. ANNE MARIE DELORT, Nolwenn Wirgot, Virginie Vinatier, Martine Sancelme, Laurent Deguillaume, *Université Clermont Auvergne*

Chemical reactions in clouds lead to oxidation processes driven by radicals (mainly $HO^{\bullet}$, $NO3^{\bullet}$ or $HO2^{\bullet}$) or strong oxidants such as H2O2, O3, nitrate and nitrite. Among those species, hydrogen peroxide plays a central role in the cloud chemistry by driving its oxidant capacity. In cloud droplets, H2O2 is transformed by microorganisms which are metabolically active [1]. Biological activity can therefore impact the cloud oxidant capacity. The present article aims at highlighting the interactions between H2O2 and microorganisms within the cloud system.

First, experiments were performed with selected strains studied as reference isolated from clouds in microcosms designed to mimic the cloud chemical composition, including the presence of light and iron. Biotic and abiotic degradation rates of H2O2 were measured and results showed that biodegradation was the most efficient process together with photo-Fenton process. H2O2 strongly impacted the microbial energetic state as shown by adenosine triphosphate (ATP) measurements in the presence and absence of H2O2. This ATP depletion was not due to the loss of cell viability.

Secondly, correlation studies were performed based on real cloud measurements from 37 clouds samples collected at the puy de Dôme station (1465 m a.s.l., France). The results supported a strong correlation between ATP and H2O2 concentrations and confirmed that H2O2 modulates the energetic metabolism of the cloud microbiome. The modulation of microbial metabolism by H2O2 concentration could thus impact cloud chemistry, in particular the biotransformation rates of carbon compounds and consequently can perturb the way the cloud system is modifying the global atmospheric chemistry [2].

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11BA.3

Revisiting Historical Trials Data on Aerosol Ingress into Buildings and Dispersion. SIMON PARKER, Suzie Abbs, Simon Batchelor, Richard Beedham, Steven Herring, Patrick Rosenvinge, *DSTL, UK*

Understanding the airborne transport of aerosol and gas phase materials and their ingress into buildings is important for assessing the risks from hazardous materials, including bioaerosols. In particular, the reduction in exposure provided by buildings can be an important factor in reducing risk. However, information on building ingress is very limited, especially for hazardous materials. This makes it difficult to validate modelling frameworks that have recently been developed to couple outdoor and indoor dispersion simulations.

A recent review has been conducted of historical experiments at Dstl, Porton Down, UK. This review coincided with the 100 year anniversary of the site and has identified a number of trials performed between 1920 and 1960 that investigated the ingress of hazardous materials into buildings. The trials examined transient concentrations in single and two storey building interiors when subjected to external challenges from a variety of gas and aerosol phase materials. The trials were motivated by the need to assess the protection offered by buildings in the event of potential aerial attack by chemical materials during the Second World War. A particularly valuable dataset relates to multiple experiments performed using the same isolated two-storey house in both an unmodified and protected form.

While subject to some limitations due to the instrumentation capabilities of the time, the data provide evidence of how the concentration profile develops and decays in indoor environments when compared to a transient period of raised outdoor concentrations. This provides invaluable information for the validation of simulations and understanding how hazardous materials infiltrate and behave in indoor environments.

During the review of historical building ingress studies, a number of dispersion experiments were identified that used aerosol phase material. These studies provide valuable information on aerosol dispersion that can be used to validate and inform the development of current dispersion models.

This paper will introduce the range of historical experiments identified, and highlight those that provide unique insights into aerosol dispersion and building ingress of hazardous materials. It will describe the experimental methodologies used and present selected results from the experiments. It will highlight conclusions of relevance to current model development and validation, but also others that are relevant to current bioaerosol hazard assessment approaches and shelter-in-place advice.

11BA.4

Indoor-Outdoor (I/O) Exchange of Bioaerosols at Various Ventilation Modes. JURATE VIRKUTYTE, Christine Uebel, Kelechi Isiugo, Michael Benjamin, Andrew Maier, Mark T. Hernandez, Sergey A. Grinshpun, Tiina Reponen, *University of Cincinnati*

People are exposed to bioaerosols both indoors and outdoors. Previous studies have typically focused on individual classes of airborne microbes. To simultaneously evaluate the indoor-outdoor exchange of bioaerosol particles, two direct Ultraviolet laser induced fluorescence instruments (UVLIF) were concomitantly deployed inside and outside of unoccupied home in summer, Cincinnati, OH. Three ventilation modes were studied: 1) windows closed, air conditioner off; 2) windows closed and air conditioner on (set at 70°F) and 3) windows opened and air conditioner off. As determined by CO_2 decay, air exchange rates were 0.15, 0.24 and 1.03 for the above ventilation modes, respectively. As judged by UVLIF, of the fluorescent particles indoors, approximately 26% were bacteria, 38% were fungal spores, and 21% were pollens or their fragments. The respective values for outdoors were 31, 29, and 25%. The total concentrations of fluorescent bioaerosol particles indoors were 17,036, 16,725, 31,143 counts per m^{-3} for ventilation modes 1, 2 and 3, respectively. The corresponding outdoor values were 58,502, 51,372 and 40,050 counts per m^{-3}. Average I/O ratios for total fluorescent particles were 0.64, 0.27 and 0.77 for ventilation modes 1, 2 and 3, respectively. Ventilation mode 2 had the lowest I/O ratios for all the bioaerosol types, except for bacteria. We hypothesize that larger I/O ratio for bacteria (0.69) in comparison to fungi (0.12) and pollen (0.08) during ventilation mode 2 can be attributed to particle size. Individual airborne bacteria cells are usually in the range between 0.5 to 1.5 µm in optical diameter, thus they remain in the air longer and are generally less efficiently filtered by the ventilation filter than their fungal and pollen counterparts. According to Spearman's correlation analysis, the indoor total fluorescent particle concentration had a significant positive correlation with fungi ($r = 0.94$, $P < 0.001$). Meanwhile, the outdoor total particle concentration had a significant positive correlation with bacteria ($r = 0.89$, $P = 0.02$) and fungi ($r = 0.83$, $P = 0.04$). However, a negative correlation was found with pollen ($r = -0.89$, $P = 0.02$). In conclusion, this study emphasizes the need for more detailed research on I/O exchange mechanisms for various bioaerosol types.

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11BA.5

Rapid Bioaerosol Exposure Risk Analysis in Typical Indoor Environments. MINFEI WANG, Haoxuan Chen, Maosheng Yao, *Peking University*

Exposure to bioaerosols can lead to adverse health effects, such as respiratory disorders, allergic diseases and toxic reactions. Some certain highly-infectious agents can pose a deadly threat to health even in a very low dose. Accordingly, it is of significant importance for sampling infectious bioaerosols with low concentration. In this study, a high flow portable bioaerosol sampler (HighBioTrap) with a sampling flow rate of 1200 L/min was used to collect air samples in three different indoor environments (subway station, hospital and student dormitory). The air samples were concentrated into small amount of mineral oil and further analyzed using real-time quantitative polymerase chain reaction (qPCR), culture, loop-mediated isothermal amplification (LAMP) and high-throughput gene sequencing technology. The results indicated that the HighBioTrap can concentrate bioaerosols efficiently. Among three typical environments, total bacterial aerosols was detected up to $6.23\times10^5/m^3$ in the hospital air samples. According to the gene sequencing analysis, subway air samples were observed to have the greatest diversity and richness of both bacterial and fungal community. Some differences were also observed among the top five genera of bacteria of all air samples collected from different environments. Using the LAMP method, we did not detect common human respiratory pathogens in the air samples collected, possibly due to lower levels. Overall, here we have developed a protocol for rapid microbial detection in a typical environment, by integrating a portable high volume sampler along with LAMP method. In the future, this method can be further used in various indoor environments for rapid pathogen detection.

Keywords: bioaerosols; high flow portable bioaerosol trap (HighBioTrap); concentrate; exposure risks

11BA.6

UV Intensity Calculated in Approximations of Clusters of Bacteria and Bacterial Spores for Predicting Viability. STEVEN HILL, Dan Mackowski, Frank Handler, Jana Kesavan, Adam Driks, David Doughty, *US Army Research Lab*

Understanding the photo-inactivation of bacteria by ultraviolet (UV) light is important in predicting and warning of biological hazards and in using germicidal UV to sanitize the air or surfaces. Bacterial spores tend to remain viable in the environment far longer than do vegetative cells. Clusters of bacteria are more difficult to inactivate with UV than are individual bacteria. Here we mathematically model Bacillus subtilis spores as homogeneous spheres and study clusters of these spheres. Each cluster of spores may be encased in an encompassing sphere of the same or different composition, or may be clean, with only air in the spaces between the spores. We use these models to better understand and estimate the distributions of UV intensities within particles containing bacteria, the shielding of some bacteria from UV, and variations of the UV intensities with wavelength. Two methods are used to calculate the UV intensities. The primary method is the multi-sphere T-matrix (MSTM) method, which provides exact solutions for the UV intensities in the spheres of the cluster. It is applicable to clusters of bacteria, with or without additional material in the spaces between the bacteria, where the individual spores or bacteria are reasonably approximated as homogeneous spheres. Because the MSTM is computationally intensive, especially for larger clusters, e.g., greater than 5-micrometer diameter, we also used a homogeneous sphere model. This model is applicable to the special case of particles formed by drying liquid droplets containing bacteria where the droplets include sufficient soluble material to cover all the spores in a cluster, and where the optical properties of the non-spore material is not too different from that of the spores. The MTSM (or a similar code capable of representing the spheres and the material in between the spores) is essential for cases where the refractive index in the spaces between the spores in a cluster is significantly different from the refractive index of the spores. Such differences are especially important when the cluster is made of clean spores, i.e., with air in the spaces between spores. Calculated intensities, using clusters containing as many as 100 spores, show that the UV exposure of individual spores within the cluster can be orders of magnitude smaller than for isolated spores under the same ambient light conditions. These effects, which are due to both absorptive and refractive shielding, are far more significant for particles in a fixed orientation, as when held on a surface. Such effects are less significant for particles rotating in air. We suggest that modeling capabilities such as these can help in predicting the time-dependence of the inactivation of bacteria exposed to UV of various intensities and spectral content. A limitation of the model is the uncertainty in the estimations of the complex refractive index of the bacteria (and of some of the other materials which may be in a cluster) at the wavelengths studied. This uncertainty is greater at wavelengths larger than approximately 290 nm, where absorption of light by nucleic acids, proteins and calcium dipicolinate no longer dominate the absorption. Other limitations at present are the assumptions that each spore is a homogenous sphere, and that reflections of UV from surfaces touching the cluster do not affect the UV inside the spores of the cluster.

11BA.7

Real-time Characterization of Airborne Bacteria Using Optofluidic Surface-Enhanced Raman Spectroscopy (SERS) Platform. JAE HEE JUNG, Jungan Choi, *Korea Institute of Science and Technology*

Bioaerosols such as viruses, bacteria, and fungal spores are closely related to human health problem both indoor and outdoor places. Their size distribution ranges from 20 nm to 100 μm which is easy to be aerosolized into the air. Due to their low settling velocities, they are suspended in the air for a long time and have the potential for spread over a wide area within a short period. Also, these properties increase the possibility of inhalation, which can amplify the potential for adverse human health effects, infectious diseases, pneumonia, asthma, and allergies. Therefore, for active disease control and to minimize bioaerosol exposure risk, there is a requirement for effective bioaerosol monitoring systems, including continuous bioaerosol sampling and rapid analysis

Recently, micro-fluidics based devices with portability and high sensitivity for detecting microorganism and fine particle have been widely developed. A new diagnostics for real-time single-cell detection based on flow cytometry technic have been introduced using target aptamer-conjugated fluorescent nanoparticles for specific cell counting methods (Chung et al., 2015). The micro-optofluidic platform was developed for quantitative analysis of bioaerosol by Choi et al. (2015). However, there is no integrated optofluidic system for qualitative measurement of bioaerosol using Raman spectroscopy with continuous aerosol sampling. Raman spectroscopy is label-free and non-destructive analysis method. Therefore, it is the proper way for molecular detection and cellular analysis.

Here, we demonstrate a micro-optofluidic platform for real-time detection and quantitative analysis of airborne microorganisms using Raman microspectroscopy. In general, the Raman signal has intrinsically weak intensity with the order of 1 photon per 10^6 incident photons which means very low sensitivity compared to Rayleigh scattering. To overcome low intensity, we employed the surface-enhanced Raman Spectroscopy (SERS) techniques using silver nanoparticles to improve Raman signal up to ~10^{11} times amplifying using plasmonic resonance effects.

In our study, the optofluidic platform involves the following three steps: (1) sampling of airborne microorganisms; (2) mixing and reacting in a microchannel for staining; and (3) real-time detection and analysis of microorganism using Raman signal. Numerical simulations were conducted for the design of micro-optofluidic platform and estimation of particle collection efficiency before the experiment. Five different microorganisms and polystyrene latex particles were introduced for the performance evaluation.

In the curved-microfluidic channel, the two-phase fluid (sampling air and collecting liquid) stably forms a stratified flow. The collecting liquid including silver colloid covers the outer wall of the channel during bioaerosol sampling. For collection, the particles are transferred from air to the liquid phase by centrifugal and drag forces by passing fluids through the curved region. The cut-off diameter of particle collection was selected controlling the air flow velocity (microfluidic air flow of 1.2 L/min showed a particle collection efficiency of ~98% at a particle diameter of 1 μm), and continuous enriched particle sampling was possible for real-time SERS measurement to identify sampled particle.

Our results indicated that the developed system represents a significant step forward as an inexpensive, simple, portable and continuous bioaerosol monitor based on the optofluidic platform.

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11BA.8

Molecular Genetic Staining Techniques for Bioaerosol Analysis in the Amazon Rainforest. MARIA PRASS, Florian Ditas, Isabella Hrabe de Angelis, Bruna A. Holanda, Oliver Lauer, Ovid Krüger, Bettina Weber, Paulo Artaxo, Eckhard Thines, Bernhard M. Fuchs, Meinrat O. Andreae, Ulrich Pöschl, Christopher Pöhlker, *Max Planck Institute for Chemistry, Mainz, Germany*

Bioaerosols, such as pollen, bacterial and fungal spores or plant fragments, can be seen as natural markers for the interaction between biosphere and atmosphere. Besides their ecological function as dispersal units of biological organisms they also influence physical and chemical processes in the atmosphere. They play an important role in cloud microphysics by acting as giant cloud condensation nuclei and ice nuclei. An extensive set of bioaerosol detection techniques is existing, however, the analysis is challenging due to their high complexity in terms of size, morphology and cell physiology. The current scientific knowledge about bioaerosols suffers from a lack of methods to individually identify and quantify these highly diverse particles in environmental samples.
Here, we present a study using a molecular genetic staining method to investigate bioaerosol composition, concentration and morphological properties in the tropical rainforest in the Amazon basin. Filter samples from three different heights (5, 60, and 325 m) at the Amazon Tall Tower Observatory (ATTO) were analyzed using Fluorescence In Situ Hybridization (FISH). FISH is based on the annealing of a specific, fluorescently labeled oligonucleotide probe to the target cell's ribonucleic acid. This way, single cells can be detected in the microbial community on filter samples via fluorescence microscopy. This is the first study based on direct visualization of bioaerosol's taxonomic diversity in a pristine rainforest.

Initial results show pronounced gradients in the rain forest boundary layer with substantially higher bioaerosol mass abundance below the forest canopy. It clearly stands out that small bioaerosol particle (1-2 µm) are more efficiently transported to higher altitudes, whereas larger eukaryotic cells (mostly fungal spores) show high abundances in the canopy space. Our results presented here are a first step towards a quantification of taxonomically resolved bioaerosol fluxes from the forest ecosystem to altitudes (i.e., cloud base height), where they become relevant for cloud microphysics.

11CA.1

The Ubiquity of Biomass Burning Particles in the Remote Troposphere. GREGORY SCHILL, Karl D. Froyd, Daniel Murphy, Agnieszka Kupc, Christina Williamson, Charles Brock, Huisheng Bian, Mian Chin, Peter Colarco, *NOAA ESRL and CIRES, University of Colorado Boulder*

It has been shown that natural aerosols provide a large contribution to uncertainty in indirect forcing, largely because forcings are referenced to the preindustrial state. Since direct measurements of preindustrial aerosol are lacking, a sound understanding of aerosol chemical and physical processes are imperative to reducing this uncertainty. Of these natural aerosol, biomass burning particles may be particularly important. Currently, the emission, transport, and removal of biomass burning particles to/from the remote troposphere is poorly constrained due to a dearth of *in-situ* observations.

In this work, we report measurements of biomass burning particles abundance during the Atmospheric Tomography (ATom) mission. During ATom, nearly continuous profiles of aerosol composition were measured by Particle Analysis by Laser Mass Spectrometry (PALMS) from approximately 150 m to 12000 m, primarily over the remote ocean. Producing the first global map of biomass burning aerosol, we find that biomass burning particles make up approximately 1/3 of the aerosol number and 1/5 of the aerosol mass in the remote troposphere. PALMS-derived mass concentrations were compared to global climate model outputs from GEOS-5 using a bulk aerosol microphysical scheme and QFED fire emissions. Sensitivity studies were conducted to determine which processes drive biomass burning particle abundance in the remote troposphere. We then explore the origins of biomass burning in the remote troposphere, and assess the importance of biomass burning particles as fire seasons extend in a warming climate.

11CA.2

Physical, Chemical, and Optical Properties of Aged Smoke Aerosols and Impacts on Boundary Layer Clouds over the South Atlantic during CLARIFY. JONATHAN TAYLOR, HuiHui Wu, Ian Crawford, Keith Bower, James Allan, Dantong Liu, Michael Flynn, Paul Williams, James Dorsey, Tom Choularton, Justin Langridge, Cathryn Fox, Michael I. Cotterell, Nicholas Davies, Kate Szpek, Hugh Coe, Jim Haywood, *University of Manchester*

We present an overview of aerosol and cloud microphysical measurements taken during the CLARIFY campaign during August – September 2017 on the UK FAAM Bae-146 Airborne Research Aircraft. CLARIFY flights targeted the semi-permanent stratocumulus deck that caps the marine boundary layer over the South Atlantic. Biomass burning in central/southern Africa lofts smoke layers up to altitudes of several kilometres during the dry season (June-September). These smoke layers descend as they travel West over the south Atlantic, eventually mixing into the boundary layer and often entraining into the cloud deck. Our observations constitute the most detailed and comprehensive set of measurements of highly aged smoke in this region, and may be used to improve constraint on aerosol and cloud radiative forcing.

28 research sorties were flown out of Ascension Island in the remote South Atlantic. Ascension is uniquely placed to receive a variety of pollution conditions; we will discuss case studies showing aged pollution in lofted layers before and after descent and mixing into the boundary layer, and contrast aerosol and cloud properties with cleaner cases. We will also discuss average and variation in properties such as organic/inorganic aerosol composition, size distribution, and black carbon mixing state in these heavily aged plumes, and the corresponding effects on aerosol optical properties.

Submicron aerosol composition was dominated by organics, which were heavily photochemically aged after several days transport time in the tropics. Inorganic composition showed temporal and vertical variation; boundary layer aerosol was acidic in mid-August and was lacking in nitrate. Later in the campaign nitrate was more prominent and at times increased with altitude. Black carbon was thickly coated throughout the campaign, though calculated coating thicknesses sometimes showed similar vertical variation with nitrate. Absorption enhancements were observed by quantifying the effect of passing particles through a thermodenuder on aerosol absorption.

Cloud properties were found to be very sensitive to the boundary layer aerosol concentrations. In clean conditions, cloud drop number concentrations (CDNCs) as low as 20/cm3 were measured. In polluted conditions these reached as high as several hundred per cubic centimetre. This difference was also accompanied by differences in the median volume diameter and drizzle concentrations, which together show a clear effect of boundary layer aerosol on cloud properties.

11CA.3

Use of Electron Tomography to Analyze the Actual Primary Particles Distribution and Agglomerate Morphology of Soot. Alberto Baldelli, STEVEN ROGAK, Una Trivanovic, *University of British Columbia*

Measuring the properties of soot agglomerates is fundamental to the understanding of their impact to the prediction of emission rates and of climate forcing of black carbon particles. Here, soot samples were collected from a large lab-scale flare of up to 80 mm in diameter with turbulent flames up to 3 m tall. The flare initial conditions vary in fuel composition, a mixture of methane, ethane, propane, butane, N2, and CO2, according to the burner diameters, 38, 51, and 76 mm. The flare exit velocity ranged from 0.5 to 1.5 m/s.

A previous literature reference showed that imaging soot agglomerates in 3D, with an electron tomography, can help to understand their complex morphology to observe details that are challenging to be determined when analyzing them in 2D. One of the findings from the 3D tomography is that soot agglomerates exhibit ring structures, in contrast to expectations from classical, perfect-sticking Cluster-Cluster Aggregation models.

The electron tomography of soot agglomerates consists of a group of 2D images taken each 2° in a range of view that goes from -70 to 70°. This study aims to use a validated code, designed for the analysis of 2D images, with the results obtained with electron tomography to determine the primary particle size distribution. Thus, the dependence of the primary particle distribution and the projected angle of the soot agglomerate is estimated.

11CA.4

Evaluation of Relative Humidity Impacts on Biomass Burning Aerosol Particle Viscosity and Volatility using a Tandem Differential Mobility Analyzer. CHRISTOPHER OXFORD, Rajan K. Chakrabarty, Brent Williams, *Washington University in St. Louis*

High viscosity of the condensed phase has been predicted to inhibit diffusion of organic species in aerosol particles[1]. The characteristic time for diffusion of particle-phase organic species could vary by orders of magnitude depending on the particle's viscosity. High viscosities would prevent evaporation of organic species, while lower viscosity would have little or no discernable impact[2]. Since vapor pressure and enthalpy measurements often use kinetic methods to characterize the aerosol, results from those measurements could be biased by particle-phase viscosity effects.

The inclusion of water in the condensed phase will reduce the particle viscosity and has been shown to reduce the characteristic time for diffusion[3]. The presence of inorganics in aerosols increases the ability of the particles to uptake water in an elevated relative humidity (90%) environment. Therefore, aerosol sources containing both inorganics and organics provide an ideal system for assessing the influence of relative humidity on primary particle phase volatility.

Flaming combustion of herbaceous plants often emits inorganic species, but the inorganics do not emit during low temperature (200 C) smoldering combustion. By varying the combustion phase (flaming vs smoldering vs mixed), we can alter the inorganic/organic content, and therefore the hygroscopicity of the aerosol. Water vapor can then be introduced to the aerosol to assess the impact of viscosity on primary emissions.

We emitted primary aerosol from the combustion of herbaceous plants and used a Tandem Differential Mobility Analyzer coupled with a Centrifugal Particle Mass Analyzer to measure the vapor pressure and enthalpy of the primary aerosol. By altering the relative humidity of the aerosol stream, we determine the impact of water on the apparent volatility of the emitted aerosol.

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[2] Shiraiwa, M. & Seinfeld, J. H. Equilibration timescale of atmospheric secondary organic aerosol partitioning. Geophys Res Lett 39, doi:Artn L24801 doi: 10.1029/2012gl054008 (2012).
[3] Shiraiwa, M., Ammann, M., Koop, T. & Poschl, U. Gas uptake and chemical aging of semisolid organic aerosol particles. P Natl Acad Sci USA 108, 11003-11008, doi:10.1073/pnas.1103045108 (2011).

11CA.5

High-temperature DMA Analysis of Wood Combustion Originated Particles. Heikki Lamberg, OLLI SIPPULA, Jorma Joutsensaari, Mika Ihalainen, Jarkko Tissari, Anna Lähde, Jorma Jokiniemi, *University of Eastern Finland*

Soot particles from combustion sources are known to have significant environmental effects. One of the major sources of soot particles is small-scale wood combustion, and there is an urgent need to develop methods to abate soot emissions from these appliances. The oxidation of soot particles in the combustion chamber is essential for the control of harmful emissions. Thus, the oxidation characteristics of wood combustion particles were studied in a high-temperature tandem differential mobility analyzer, which contained particle classification, a high-temperature reactor and scanning mobility particle sizer for measuring any possible changes in particle size taking place inside the reactor.

Particles were generated using a pellet boiler, which was operated with low load mode to increase the proportion of soot within the particles, and a wood stove. The aerosol was diluted using a porous tube diluter and an ejector diluter, and led to a sampling chamber that stabilized the small variation in the particle concentration generated by the combustion process. Sample was led from the chamber to a differential mobility analyser, which classified particles to a certain size class (40 nm, 100 nm or 200 nm). This was followed by a temperature-controlled laminar flow reactor. The oxygen concentration in the reactor was close to atmospheric concentration because of the sample dilution. Temperature inside the reactor tube was varied up to 1000 °C and the changes in the particle size were measured using a scanning electrical mobility analyser (SMPS, TSI Inc.). Particle samples were additionally collected for chemical analysis and electron-microscope analysis and transmission electron microscopy. Finally, kinetic parameters for assessing wood combustion soot oxidation under conditions representing the post-combustion zone of small appliances were derived.

Chemical analyses of the PM_1 samples showed that about 50% of the PM_1 was composed of EC and about 10% of OC. The most abundant inorganic species were potassium, sodium, sulphate, chloride and nitrate. Their total share was about 25% of the total PM_1.

There was no considerable oxidation of the wood combustion particles below 400 °C. In all particle sizes in pellet combustion, the minimum particle sizes were reached at 750 °C, while wood stove particles were not fully oxidized at 900 °C. At 750 °C, both 100 nm and 200 nm pellet combustion particles reached GMD 28 nm, and 40 nm particles reached GMD 19 nm. At 900 °C there was no particle mode left; soot particles in 100 nm size were oxidized at 750 °C and once temperatures reached 900 °C, also inorganic particles were evaporated. Furthermore, the double mode in 600 °C indicated that there were two types of particles in the 100 nm size, for which the oxidation rate was different.

This difference is a result of the high alkali metal content in pellet combustion particles, which presumably leads to catalytically enhanced oxidation of soot particles. However, the wood stove particles with low alkali metal content also had lower oxidation temperatures compared to previously studied diesel combustion particles. According to the fitting parameters, about 70% particle reduction could be achieved with one second residence time at 800 °C. These results can be utilized in the development of strategies and technologies to abate soot emissions from small-scale wood-fired combustion appliances.

11CA.6

Speciated Molecular Emission Factors and Volatilities of Biomass Burning Aerosols from Western US Forest Fuels.

COTY JEN, Lindsay Hatch, Nathan Kreisberg, Christos Stamatis, Vanessa Selimovic, Robert J. Yokelson, Kelley Barsanti, Allen H. Goldstein, *University of California, Berkeley*

Wildfires are predicted to become larger and more frequent in many temperate and boreal forests, primarily due to changing climate (e.g. longer springs and summers, earlier snow melts, and prolonged droughts). Wildfires, and biomass burning more generally, are a dominant source of carbonaceous aerosols into the atmosphere, and represent a large fraction of gaseous volatile organic compound (VOC) emissions globally. It is predicted that > 50% of the non-methane organic chemicals from biomass burning are intermediate and/or semi volatile compounds (I/SVOCs) that can further react and partition into aerosol particles. The identities and quantities of most of I/SVOCs remain unknown, leading to uncertainty in predicting the extent to which wildfire smoke impacts air quality, human health, and the environment now and in the future.

This study examines the chemical identities and volatilities of molecules found in smoke produced from laboratory fires during the FIREX Fire Laboratory (US Forest Service, Missoula, MT) campaign and prescribed burning in the foothills of the Sierra Nevada (Blodgett Forest Research Station, CA). Filter and sorbent tube samples of fresh emissions were collected from the smoke stack at the Fire Lab for a variety of trees, ground cover, and shrubs typically found in the Western US, a region susceptible to large scale wildfires. These observations were then compared to real fire samples collected from prescribed burns conducted at Blodgett Forest Research Station. Smoke samples were collected using an unmanned aircraft system (UAS) that flew 25-50 m above the burns and a ground-base station. A two-dimensional gas chromatogram coupled to an electron impact or vacuum ultra violet light high-resolution time of flight mass spectrometer (GCxGC EI/VUV HRToFMS) was used to speciate and quantify the I/SVOCs in collected smoke samples from both campaigns. In addition, vapor pressures and log of the effective saturation concentrations (log C*) for all ~3000 observed compounds were estimated from their retention times based on fit to known standards. Results indicate that smoldering burns (low modified combustion efficiency, MCE) from rotten logs and duff fuels produced the highest emission factors and likely produce the vast majority of smoke during wildfire burns. Higher MCE values or more flaming conditions, produced lower emission factors for all observed compounds across all fuel types. In addition, we combined GCxGC measurements of sorbent tubes and filters to quantify amounts of each compound class across the volatility groups. These results can be used in the future to construct partitioning models and help predict aerosol chemistry.

11CA.7

Photochemical Aging of Light-Absorbing Biomass Burning Aerosol Selected by Volatility. ELIJAH SCHNITZLER, Rachel Hems, Jonathan Abbatt, *University of Toronto, Toronto, Canada*

Brown carbon (BrC) aerosol from biomass burning (BB) has significant but poorly-constrained effects on climate. For example, absorption of solar radiation by BrC may increase downwind of a source if secondary chemistry produces more chromophores; in contrast, absorption may decrease if bleaching of primary chromophores predominates. Recently, the reactivity of ambient brown carbon, with respect to atmospheric aging, has been shown to decrease as the molecular size of the constituent chromophores increases. It is also known that the volatility of an organic aerosol component generally decreases as molecular size increases. Here, we investigate the photochemical aging of BrC generated from low-temperature BB of pine and selected by volatility using a thermo-denuder at a range of temperatures. Particles were generated by passing air through a heated (300 °C) flow tube containing pine. Subsequently, particles were passed through a diffusion dryer, a trace gas denuder containing activated carbon, and a thermo-denuder before being injected into a smog chamber, where they were exposed to OH radicals at a relative humidity of about 60%. Aerosol absorption and scattering coefficients were measured using a photo-acoustic spectrometer with an integrated reciprocal nephelometer. Based on the experimental single scattering albedo and particle size distributions, measured using a scanning mobility particle sizer, along with Mie theory calculations, the initial complex refractive indices of the treated particles were derived. Observed trends in the optical properties of the particles were compared to hypothetical trends that would be expected for the experimental size distributions and a constant refractive index. For each thermo-denuder temperature, deviations from the hypothetical trends provide insights into the dependence of BrC reactivity on the volatility of the constituent chromophores.

11CB.1

Interpretation of UV-Visible Absorption Measurements of Flame-synthesized Carbon Nanoparticles by Molecular Modeling. DONGPING CHEN, Hai Wang, *Beijing Institute of Technology*

Recent UV-Visible absorption spectral analyses of a series of flame-synthesized carbon nanoparticles show that these particles exhibit the quantum confinement behavior. The measured, apparent optical bandgaps increase with a decrease in particle size; they lie in the range of 0.7 to 1.8 eV for particles with median mobility diameter ranging from 3 to 13 nm. To interpret these results, we carried out molecular dynamics/electronic structure calculations for homogeneous clusters of polycyclic aromatic hydrocarbons (PAHs) including ovalene, coronene, pyrene and naphthalene. PAH clusters were built using molecular dynamics method followed by a search of minimum HOMO-LUMO gap over sampled configurations. The HOMO-LUMO gap was computed from the difference in energies between the HOMO and LUMO Kohn–Sham orbitals at the B3LYP/6-31G(d) level of theory. It was found that the morphology of PAH clusters (< 2 nm) have a large impact on the HOMO-LUMO gap; a T-shaped configuration always leads to a lower gap value. Similarly to experimental observations, the HOMO-LUMO gap of PAH clusters is found to be a function of the particle size. By extrapolating the correlation between HOMO-LUMO gap and particle size, the difference in the bandgap of a single PAH molecule and the bulk PAH is 1.4+/–0.2 eV. From the measured optical bandgap values, the largest PAH within a particle of a given size may be estimated. For a particle 3 nm in diameter with a measured bandgap of 1.8 eV, the largest PAH is around the size of ovalene. For a particle 10 nm in diameter with a bandgap value of 0.7 eV, the largest PAH corresponds to 40 carbon atoms. These estimates were made with the assumption that the carbon nanoparticles do not contain any oxygenates. If oxygenates are present, the estimated, largest PAH size is expected to decrease. Overall, the results suggest that molecular modeling coupled with UV-vis absorption spectroscopy is a valuable approach to estimating the largest PAH component in carbon nanoparticles.

11CB.2

Polyaromatic Hydrocarbon Dimerization Rates: Results from ReaxFF Molecular Dynamics. EIRINI GOUDELI, Christopher Hogan Jr., *University of Minnesota*

Collisions dynamics between carbonaceous molecules in combustion systems are what ultimately govern soot nanoparticle formation (nucleation) and growth. When collisions lead to binding/reaction between molecular monomers, the result is a nanocluster, which may in turn grow collisionally. Nanocluster collisional growth rate calculations are often based upon simplified approaches, in which the binding rate (collision and sticking rate) is calculated assuming hard-sphere potential interactions between colliding entities and assuming a sticking efficiency of 100%. However, this approach neglects both potential interactions between monomers and nanoclusters and does not accurately consider incomplete kinetic energy to internal energy exchange during collision.

In particular, reactions between polyaromatic hydrocarbons (PAHs) are prominent in the earliest stages of soot nanoparticle formation. Here, we examine the dimerization rate of common PAH molecules (e.g., naphthalene, pyrene, coronene), that lead to formation of nascent soot, via reactive molecular dynamics using ReaxFF C-H potentials. In simulations, PAH clusters are equilibrated (at a predefined temperature) and collide with another PAH cluster of same kind with a specified velocity and impact parameter. A map of the sticking (or reaction) probability between such molecules is obtained ab initio as function of velocity and impact parameter. In simulations, we find that high relative velocities for PAH clusters lead to non-sticking (bounce, dissociation). Integration over the reaction probability for the above impact parameters and velocities (in accordance with the Maxwell-Boltzmann distribution) yields accurate reaction rate coefficients of dimerization that are compared to experiments. Furthermore, we discuss how these rates vary with temperature and cluster size. An effective collision efficiency is proposed for PAH clusters of different mass.

11CB.3

Laboratory Flames under Investigation: Identifying Trends in Combustion When Mass spectrometry Meets Statistical Analysis. Cornelia Irimiea, Alessandro Faccinetto, Xavier Mercier, Ismael Kenneth Ortega Colomer, Eric Therssen, CRISTIAN FOCSA, *ONERA*

Combustion attracts a high scientific interest due to the number of applications that range from power generation to automotive and airplane engines. In general, combustion-based technology poses significant challenges when it comes to maximize the performance while reducing emissions. Incomplete combustion processes release, among other pollutants, soot particulate into the atmosphere. The environmental impact of these by-products have led to the development of experimental techniques that contribute to a better understanding of the fundamental physical and chemical combustion processes. The characterization of adsorbed volatile organic compounds on these particles may help to track the emitting source and to identify the processes leading to their incomplete conversion.

For this reason we pay special attention to simpler combustion sources, by investigating the formation of large hydrocarbons inside laboratory flames at different combustion stages (from below the soot inception up until the oxidation regions). In this context, two methane low pressure premixed flames are stabilized in conditions that result in similar concentration profiles of known polycyclic aromatic hydrocarbons (PAH), and molecular clustering leading to soot nucleation beginning at the same reaction time, or equivalently at the same height above the burner (HAB). After the soot inception zone, the gas phase and particulate matter coexist all along the flame height for the two premixed flames. Alternatively two methane diffusion flames are stabilized at atmospheric pressure in similar aerodynamic conditions. However, in stark contrast to the previous case in which soot and molecular precursors coexist all along the reaction coordinate, the diffusion flames show a net stratification of the soot (downstream the flame tip) and molecular precursors (near the fuel injection point) regions that are sufficiently far to be probed independently and with little interference from each other.

Many theoretical and experimental evidences point to the role of PAH as soot precursors. Therefore, understanding their chemistry will lead to a better understanding of the soot formation process. This work proposes a unique approach and methodology for the characterization of soot particle surface and condensable gas phase collected from laboratory flames at different (HAB). Secondary ion mass spectrometry (SIMS) is used for identifying the compounds adsorbed on the surface of soot samples. The high mass resolution ~7000 allows attributing PAH and oxygenated hydrocarbons as the main contributors to the chemical reactions leading to soot nucleation. Additionally, statistical methods as principal component analysis (PCA) and hierarchical clustering analysis (HCA) are used for data interpretation. These detailed analyses provide an innovative approach when dealing with complex mass spectra of soot. Once the sampling conditions were taken into account, we succeeded to identify similar conditions of soot evolution in flames where the growth/oxidation mechanisms exist (for one premixed flame and the two diffusion flames). Multivariate data analysis aids to separate the species involved in the soot nucleation phase suggesting that a broad range of PAH are participating to this process.

11CB.4

Size, Effective Density, Volatility, Morphology, and Internal Structure of Soot Particles Generated from Large-Scale Turbulent Diffusion Flames. MOHSEN KAZEMIMANESH, Ramin Dastanpour, Alberto Baldelli, Melina Jefferson, Alireza Moallemi, Kevin Thomson, Matthew Johnson, Steven Rogak, Jason S. Olfert, *University of Alberta*

Flares in the oil and gas industry are an important source of particulate emissions. Global gas flaring volume was approximately 150 billion m^3 in 2016; however, very little is known about the physical, chemical, and optical properties of particle emissions from flares. To study these properties, a turbulent diffusion flame was set up at Carleton University Lab-scale Flare Facility which allowed controlled experiments on flames up to approximately three meters tall at fuel gas flow rates up to ~250 SLPM (standard litres per minute at 0°C and 101.325 kPa). Size distribution, effective density, volatility, morphology, and internal structure of soot particles generated from large-scale turbulent diffusion flames were characterized under various fuel composition and exit velocity conditions. Three different burner sizes with a diameter of 38.1, 50.8, and 76.2 mm were used in this study. The fuel exit velocities at the burner tip were 0.5, 0.9, and 1.5 m/s and the fuel flow rates were adjusted accordingly for each burner size, which resulted in a range of flow rates from 60.5 to 246.2 SLPM. Three different fuel mixture compositions (light, medium, heavy) were tested which resembled Alberta flare gas composition. The fuel gas mixture had 6 components (i.e., C1 to C4 alkanes, carbon dioxide, and nitrogen) and the mole fraction of methane in the light, medium, and heavy composition was 0.925, 0.866, and 0.769, respectively.

Combustion products were diluted by the ambient air on the order of ~20:1 to ~120:1 as they were drawn in the collecting fume hood and insulated duct using a variable speed fan. Size distributions of soot particles were measured using a scanning mobility particle sizer (SMPS), sampling from the duct and after the sample was further diluted by a factor of ~10:1 using an ejector diluter. Mass-mobility relations and effective densities of soot particles were determined using a tandem arrangement of a differential mobility analyzer (DMA), a centrifugal particle mass analyzer (CPMA), and a condensation particle counter (CPC). The volatility of particles was studied by adding a catalytic stripper (denuder) between the DMA and the CPMA. Morphology and internal structure of soot particles were studied using transmission electron microscopy (TEM) and Raman spectroscopy, respectively.

Results showed that the total particle number per unit mass of fuel ranged from 1.64×10^{14} kg^{-1} fuel to 9.08×10^{14} kg^{-1} fuel corresponding to light fuel mixture burned in the 76.2 mm burner with exit velocity of ~0.9 m/s and heavy fuel mixture burned in the 50.8 mm burner with exit velocity of 0.5 m/s, respectively. Particle size distribution changed noticeably with the fuel mixture composition; i.e., the particle median diameter was 66, 82, and 92 nm for light, medium, and heavy mixtures, respectively. Mass-mobility and effective density results showed that the average mass-mobility relationship was in good agreement with previously reported values for the mass-mobility of particles from different combustion sources in the literature. The results also showed that the mass fraction of volatile coating on the soot particles was negligible. Previously developed relations between effective density and primary particle size work well for the soot particles of this study. Raman spectroscopy indicated similar nanostructure for the studied fuel compositions. It may be possible to use a simple morphology model for all the conditions investigated in this study.

11CB.5

Thermophoretic Collection of Soot Samples Taken from within a Co-Flow Diffusion Flame. JOCHEN A.H. DREYER, Maurin Salamanca, Jethro Akroyd, Sebastian Mosbach, Markus Kraft, *University of Cambridge*

Soot is the second biggest contributor to climate change after CO2 and has adverse effects on human health, making its mitigation a major field of academic and industrial research. Deepening our understanding of soot formation requires detailed information regarding the soot composition, size, and morphology as a function of fuel structure and combustion conditions. Some powerful and frequently used tools for soot characterisation are electron microscopy, Fourier-transform infrared spectroscopy (FTIR), or Raman spectroscopy. All of these techniques require soot collection under well-defined conditions to assure that the collected sample is representative of the soot in the combustion system.

Laminar flames are commonly used to study soot formation in a simplified version of real combustion systems. Soot aerosol samples from within the flame can be taken by drawing a small amount of aerosol through an orifice and immediately diluting it with an inert gas to quench chemical reactions and prevent further particle growth. Some reported methods to collect soot samples from such aerosols are filtration or micro-orifice uniform deposition impactors (MOUDI).

The aim of this work is the development of a thermophoretic nanoparticle collector that facilitates soot collection from an aerosol stream taken from within the flame. The advantage is that existing equipment for taking and diluting the sample can be used and that such a device could be used in conjunction with other devices such as a SMPS or DMS. As opposed to filtration with additional pressure drops in the sampling lines, which further increase with collection time, the thermophoretic collection does not require adjustment of the sample dilution devices. The challenge is the relatively high flow rates frequently encountered when flame samples are quenched and diluted.

Different parameters for the thermophoretic collection were explored, namely the gap separating the hot and cold plate, their temperature difference, and the sample collection time. We demonstrate how a DMS500 can be used to take samples from within a flame to measure the soot particle size distribution while a fraction of the soot is simultaneously deposited on a substrate. This approach facilitates the direct correlation between the location in the flame where the sample was taken, the measured particle size distribution, and the results obtained from characterising the collected soot layer. Such information provides valuable insight into soot composition and formation during hydrocarbon combustion.

11CB.6

Soot Nucleation and Chemical Evolution during Combustion. K. Olof Johansson, Farid El Gabaly, Paul Schrader, Matthew Campbell, HOPE MICHELSEN, *Sandia National Labs*

There are substantial gaps in our understanding of the first steps in soot formation, growth mechanisms, and chemical evolution during combustion. The first steps in soot formation involve the transition of gas-phase hydrocarbon precursors to physically or covalently bound complexes that are sufficiently stable and long-lived to initiate rapid heterogeneous nucleation and particle growth. These complexes are known as “incipient particles”, and the search for their nucleation and growth mechanisms is a subject of active research. These incipient particles initiate further nucleation and particle growth by coalescence, generating liquid-like hydrocarbon particles, which eventually reach sizes in the range of 10-50 nm, known as “primary particles”. As these particles grow, they also lose hydrogen, solidify, and agglomerate into loosely bound clusters. Under high-temperature conditions, they become graphitic, covalently bound aggregates with a dendritic structure. Soot aggregate sizes, primary-particle sizes, and volume fractions grow as particles age in the flame. At high temperatures in the presence of oxygen, the aggregates fragment, and the primary-particle sizes and volume fractions decrease through oxidation. There is a poor understanding of the mechanisms by which particles undergo these transitions and the parameters that influence them.

We have coupled multiple in situ and ex situ particle diagnostics to study the evolution of soot composition and fine structure, i.e., maturity level, in atmospheric laminar premixed and diffusion flames. We have used aerosol mass spectrometry using single-photon vacuum ultraviolet photoionization (VUV-AMS) to provide information about gas-phase precursors involved in incipient particle nucleation and availability of gas-phase species to adsorb to the particle surface during particle growth. We have used laser-induced incandescence (LII), coupled with laser extinction, to provide information about soot volume fraction and maturity level of the bulk primary particle, and X-ray photoelectron spectroscopy (XPS) to provide complementary information about particle-surface maturity level 10. XPS is sensitive to the chemical environment of atoms in a sample, providing measures of atomic composition, surface functional groups, and electronic structure, including carbon hybridization. At a photon energy of 1,253.6 eV, the mean electron escape depth in graphite is ~1-2 nm, making XPS particularly surface sensitive. This surface sensitivity is a good complement to the bulk sensitivity of LII.

The results demonstrate that the bulk material and the particle surface evolve separately in the flame. Increased soot-maturity level is associated with increased long-range order of the particle fine structure. This increased order leads to an increase in the absorption cross section in the visible and near infrared and a shift of the absorption to longer wavelengths with increasing maturity level of the bulk particle. These trends result in a decrease in the dispersion exponent and increase in the absorption cross section scaling factor, as inferred from LII measurements. LII measurements demonstrate that bulk-maturity level increases with height-above-the-burner (HAB) until it reaches a plateau in the center of the flame at the maximum in the soot volume fraction. Bulk-maturity level only slightly decreases as soot is oxidized at larger HABs. Increased maturity level also leads to an increase in long-range sp2 hybridization. XPS measurements of the sp2/defect ratio demonstrate an increase in soot surface-maturity level with increasing HAB, but the surface-maturity level increases more gradually with HAB than the bulk-maturity level. Whereas the bulk-fine-structure order decreases slightly in the oxidation region, the surface order decreases dramatically, indicating that oxidation occurs preferentially at the surface under these conditions.

11CB.7

Direct On-line Measurement Of Soot Oxidation Reactivity. REINHARD NIESSNER, Alexander Rinkenburger, Christoph Haisch, *Technical University of Munich, Germany*

Diesel soot is one of the major pollutants in the world and is classified as carcinogenic. Soot is theorized to have the second largest impact on global warming after CO2. In North America and Europe, soot is mainly emitted by diesel engines, which are equipped with particulate filters to minimize emissions. Regeneration of these filters is done by oxidation (combustion) of the soot. Uncatalyzed oxidation requires temperatures > 600 °C (5-10 Vol.-% O2 in N2), resulting in poor fuel efficiencies. Catalysts, i.e. as additives, can lower these temperatures significantly. As we have shown before, not only toxic Ferrocene- or Ce-based compounds are suitable, but also cheap, inorganic and most likely non-toxic salts. Usually, soot oxidation reactivity is derived from temperature-programmed oxidation (TPO) measurements, microscopic techniques (i.e. HRTEM, SEM), Raman microspectroscopy (RM) or other spectroscopic techniques. Most of these techniques need collected (filter) samples, are time-consuming and costly, and sometimes fail to characterize certain soot samples. So, there is definitely a need for fast and on-line methods to characterize the oxidation reactivity of soot.

Our solution to this problem essentially consists of an in-house built propane/air diffusion burner to generate soot model aerosols and a custom-built oven to thermally treat these aerosols in relation to a reference. We employed several detection systems after the oven, namely two scanning mobility particle sizer setups (SMPS), an infrared spectrometer (FTIR) and photoacoustic spectrometers (MSS, QuadPASS).

The setup was first characterized using two SMPS systems in parallel and let us to the conclusion that mean diameters are a good criterion for soot oxidation reactivity. We could also show that there is a clear, temperature-dependent decrease in mass concentrations as measured by the photoacoustic spectrometers. Soot containing salt shows earlier and faster oxidation compared to pure propane soot, which is consistent with the TPO results. In fact, we do not even need to observe full temperature programs like in the TPO measurements, but can derive parameters related to the soot oxidation reactivity very fast and on-line by single-temperature measurements. This results in a huge improvement of measurement times, enables us to follow transient systems almost in real time and gives rise to new possibilities regarding particle emission reductions.

11CB.8

Flame Generated Soot Nuclei: The Asymmetries in Collision Charging evidenced by High-Resolution (APi-TOF) Mass Spectrometry. FRANCESCO CARBONE, Manjula Canagaratna, Andrew Lambe, John Jayne, Douglas Worsnop, Alessandro Gomez, *Yale University*

Flame products were sampled with a horizontal tube probe from a well-characterized, moderately sooting premixed flame of an ethylene/air mixture with a C/O ratio of 0.69. The samples were quickly diluted in a nitrogen stream seeded with bipolar ions generated by a radioactive source. Diluted and partially charged soot nuclei and precursors were analyzed in a mass-to-charge ratio range up to 2000 using a highly sensitive Atmospheric Pressure Interface Time-of-Flight (APi-TOF, Tofwerk AG) Mass Spectrometer. The high mass accuracy and resolving power (in excess of 3000) of the measurements allowed for the accurate determination of the mass defect distributions of the sampled material that relates to its composition and charge distributions. Analyses were performed at several heights above the burner (HAB) of both positively and negatively charged material. Additionally, the type and concentrations of ions seeded in the dilution nitrogen was varied using two different radioactive sources to investigate the effect of collision charging. Results clearly show an asymmetry in the composition and in the collisional charging efficiency of material detected in different polarities. Materials acquiring a positive charge consistently have a larger content of hydrogen and is detected in significantly larger amounts as compared to materials with negative charge. Furthermore, the comparison of results using two different radioactive sources evidenced that the fraction (more properly, ion attachment efficiency) and the composition of detected materials is sensitive to the number and type of ions used for collisional charging. These findings call for a deeper investigation of the collisional charging mechanisms of flame-generated materials in the sub 2nm dimensional range. Clarification of these mechanism would allow for the quantitative determination of composition and concentration of the originally neutral material generated in the flame.

11HA.1

Online Analysis of Volatile Organic Gases Released from Bronchial Cells upon Aerosol Deposition as a Diagnostic Tool for Metabolic Processes. LAURE-ESTELLE CASSAGNES, Zaira Leni, Alexander Håland, Liang Zhu, David Bell, Urs Baltensperger, Imad El Haddad, Armin Wisthaler, Marianne Geiser, Josef Dommen, *Paul Scherrer Institute*

Air pollution has been recently estimated to cause about 4.3 million deaths per year and 123 million years of life lost [1]. Particulate matter contains chemical species such as transition metals (Fe, Cu, Mn…), quinones, organic peroxides and elemental carbon that may lead to oxidative stress at the inner surface of the lungs. However, the link between the chemical composition of particulate matter (PM) and the adverse health outcome in humans remains unclear and there is a need to develop pulmonary oxidative stress biomarkers that could be used as measures for impaired health by air pollution in medical practice or in epidemiological studies.

Many volatile organic compounds (VOC) are produced in the human body and emitted through exhalation or excretion through the skin, in the feces and in urine. The elaborations of specific marker compounds or metabolic profiles in the human breath as indicator of diseases have become a hot research topic in medical diagnostics. Proton transfer reaction mass spectrometry (PTR-MS) is commonly used for clinical analysis of gas exhaled by humans, since it is a fast, direct and non-invasive method [2]. However the literature regarding the use of PTR-MS on cell cultures is very scarce and not related to air pollution toxicity.

We aim to exploit the potential of PTR-MS on VOCs released from bronchial cells (BEAS-2B cell line) placed in an exposure chamber allowing deposition of substances either by injection or from a continuous air flow [3]. In a first set of experiments, cells were exposed to model compounds: H2O2, copper (Cu(II)), 1,4-naphthoquinone (1,4-NQ) and a combination of Cu(II) and 1,4-NQ. The compounds were injected at the air-liquid interface of the cell cultures at stable temperature and humidity and thereafter the profile of VOC emission was recorded. In a second set of experiments, cells were exposed to fresh and aged secondary organic aerosols produced in a smog chamber. In parallel, the cytotoxicity of these compounds was assessed with the LDH assay and the intracellular oxidative stress measured by using DCFH.

This innovative setup highlighted differences in the profile of VOCs released by the cells after treatment compared to the controls. The results obtained will allow us to better understand the cellular defense pathways towards aerosols leading to the release of small molecules. In addition there will be increased knowledge about the metabolism of PM by cells and biomarkers of pulmonary oxidative stress for medical applications will likely be identified.

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11HA.2

Deposition of Length-classified Glass Fibers in a Replica of Human Airways. FRANTISEK LIZAL, Miloslav Belka, Jakub Elcner, Jan Jedelsky, Ondrej Misik, Jan Tuhovcak, Miroslav Jicha, *Brno University of Technology*

Inhalable fibers form a specific group of particles, which are provably, or potentially toxic for humans [1]. A few studies applied computational fluid and particle dynamics (CFPD) calculations for prediction of localised deposition of fibers [2]. However, obtaining reliable experimental data for validation represents significant problem for all teams performing numerical simulations.

A realistic replica of human airways has been developed at Brno University of Technology. The identical geometry exists as a physical replica for experimental work and as a digital geometry for numerical simulations [3].

The results on flow and deposition of spherical particles were published in [4]. In this contribution we introduce measurement of deposition of length-classified fibers.

Experimental setup

The measurements setup was described in detail in [5]. Glass wool (Johns Manville JM 100/475) was crushed and sieved to produce fibers with a density of 2.56 g/cm3 and diameter of 1.03 ± 0.45 µm. The fibers were classified using a dielectrophoretic classifier, mixed with clean air, and sucked into the replica. Three steady inhalation flowrates (15, 30 and 50 L/min) were measured. Counting of fibers was performed by a combination of manual and automated counting [5].

Results and discussion

The deposition fraction increased with an increasing flow rate, and the total deposition fractions in the replica were 0.7%, 1.9% and 4.6% for the inspiratory flow rates of 15, 30, and 50 LPM, respectively. A slightly higher deposition fraction was detected in the oral cavity and in the complex segments. Moreover, segments in the right lung that encompassed a bifurcation in the fourth generation had a noticeably higher deposition fraction for higher inspiratory flow rates.

A comparison of deposition fractions for fibers and spherical particles confirmed that fibers deposit less effectively than spherical particles of the same Stokes number. The results of local deposition fraction, efficiency and density are available for validation of numerical simulations performed on the identical airway geometry.

Acknowledgement

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11HA.3

Atmospheric Evolution of Biomass Burning Organic Aerosol: Implications to Oxidative Potential. JENNY P.S. WONG, Maria Tsagaraki, Irini Tsiodra, Nikolaos Mihalopoulos, Kalloipi Violaki, Maria Kanakidou, Athanasios Nenes, Rodney J. Weber, *Georgia Institute of Technology*

Oxidative stress, an imbalance of Reactive Oxygen Species (ROS) production and antioxidant defenses, is one of the proposed toxicology mechanism underlying the adverse health effects associated with aerosol inhalation. While there are growing research efforts to characterize the oxidative potential (ability to generate ROS) of aerosols from different sources, less attention have been paid to assess whether the oxidative potential of aerosols evolve throughout atmospheric transport. Through a combination of field observations and targeted laboratory studies, the objective of this work is to investigate whether atmospheric aging processes can transform the oxidative potential of biomass burning organic aerosols (BBOA). Analysis of ambient filter samples collected in Crete, Greece, during the fire seasons of 2016 and 2017, suggests that the oxidative potential of BBOA was quickly transformed in the atmosphere, on the timescale of hours. To better understand which atmospheric aging processes are responsible for these ambient observations, the effect of various chemical aging processes (oxidation by OH and photolysis) on the oxidative potential of BBOA are systematically investigated in the laboratory. Collectively, results suggest that certain toxic chemical components may be long-lived in BBOA and likely an important contributor to the toxicity of ambient aerosols on a regional scale.

11HA.4

Development of a Physiologically Relevant On-Line Chemical Assay to Quantify Aerosol Oxidative Potential. STEVEN J. CAMPBELL, Daniel Lienhard, Battist Utinger, Angharad Stell, Suzanne E. Paulson, Markus Kalberer, *University of Cambridge*

It is currently estimated that up to 0.3 million premature deaths per year in Europe and 2.1 million deaths worldwide are the result of exposure to ambient particles with an aerodynamic diameter less than 2.5 µm ($PM_{2.5}$). However, the identification of the physical and chemical particle properties responsible for these observed adverse human health effects remains a challenge. Toxicological studies suggest that some of the observed adverse health effects derive from the occurrence of reactive oxygen species (ROS) and other oxidising particle components in cells, added directly through inhalation of PM or formed by reactions of particle components *in vivo*.[1] Oxidising, particle-phase components include a wide range of chemical species such as transition metals (*e.g.* iron, nickel and copper), a range of organic compounds including polyaromatic hydrocarbons (PAHs), quinones, peroxides and radicals, complicating their analysis.

In order to protect the body against these oxidising species, lung cells generate antioxidants such as ascorbic acid (AA) which are present in the respiratory tract lining fluid (RTLF); these anti-oxidants act as the first line of defence against oxidising components in aerosol particles. When these antioxidants are depleted (defined as oxidative stress), a number of cellular responses occur, including inflammatory reactions.

Offline methods have been developed previously to characterise oxidising particle components by quantifying the decrease of antioxidants.[2] These methods are based on the analysis of filter extracts sampled typically for several hours to days. The time delay between sampling and analysis in these off-line methods, which might be hours to days, may result in an underestimation of oxidising particle component concentrations or adverse health effects as some of the more reactive species might be converted to more stable compounds before analysis. In addition, the effect on composition caused by the filter extraction remains uncertain.

In this work, a new on-line method to quantify the oxidation of ascorbic acid in synthetic RTLF was developed by adapting an existing home-built instrument, which quantifies ROS based on a different reaction system (DCFH)[3]. This new instrument combines the advantages of on-line measurements (*i.e.* high time resolution of a few minutes) with the more physiologically relevant assay to estimate health-relevant oxidising aerosol properties. The applicability of this method to the oxidation of ascorbic acid by secondary organic aerosol (SOA) generated from the ozonolysis of α-pinene in a flow tube is demonstrated. The instrument response to particles containing a mixture of SOA and iron sulphate seed particles was also investigated, illustrating a synergistic enhancement of the oxidation of ascorbic acid when organic SOA and iron are sampled simultaneously, compared to SOA and iron sulphate particles separately.

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11HA.5

Lipopolysaccharide-mediated PM2.5 Dose-dependent Inflammatory Effects. FANGXIA SHEN, Fobang Liu, Xiangyu Zhang, Jing Li, Kira Ziegler, Ting Zhang, Tianle Zhu, Manabu Shiraiwa, Haijie Tong, Maosheng Yao, Ulrich Pöschl, Kurt Lucas, *Beihang University*

China has experienced frequently serious haze weather in recent years. Strong association between haze events and respiratory as well as cardiovascular disease was reported. Although fine particulate matter (PM2.5) was shown to play a crucial role in the higher incidence and exacerbation of respiratory diseases, the key underlying mechanisms are still not well understood. In our study, PM2.5 samples were collected during a haze period in winter 2016 of Beijing, China. Characterization of the PM2.5 samples were performed, including ions, metals, redox activity and particle-bound LPS. We measured inflammatory cytokine releases from human macrophages that were exposed to the water elution of PM2.5 from distinct days. Additionally we mixed (spiked) these PM2.5 extracts with lipopolysaccharide (LPS), to mimic the inflammatory conditions in sick individual's respiratory tract with a high bacterial load. Differential cellular inflammatory signals, i.e., interleukin 8 (IL-8), IL-1B and tumor necrosis factor (TNF), were observed upon exposure to the PM2.5 from same volume of air but from distinct days at sub-toxic levels. Compared to the macrophages treated with PM2.5 alone, up to 13-folds more IL-8 were released from macrophages treated with PM2.5 spiked with LPS (100 pg/mL). Moreover, changes in the expression of oxidative stress-related genes were observed to depend on PM2.5 mass levels. When spiked with LPS at 100 pg/mL, 2.5-folds higher up-regulation of the gene superoxide dismutase 2 (SOD2) was observed for the sample collected from polluted day compared to that from clean day. Our results suggest that particle-bound LPS as well as lung-resident LPS along with other constitutes mediates the PM2.5-related inflammatory effects, thereby contributing to the deterioration of existing chronic respiratory disease, like COPD. This work highlights the need to consider the biological fraction of PM2.5 such as LPS when assessing its health effects.

11HA.6

Waterpipe Tobacco Smoke Toxicity: The Impact of Pipe Height and Hose Characteristics. KAREN K. BERND, Hannah Stadtler, Jenna Reed, Alexander Dawes, Emilie Uffman, Mary Catherine Thomson, Cindy DeForest Hauser, *Davidson College*

Waterpipe tobacco smoking continues to show increasing popularity, especially among individuals between 18 and 24 years old. The waterpipe tobacco smoke (WTS) produced is mixture of UFPs formed from the combustion of the charcoal heat source and volatilization and humidification of the tobacco +humectant +flavoring substrate known as shisha or mu'assel. As such, variables in the height of the waterpipe and length and composition of the hose would likely affect the particles produced. In this study, we focus on the effects of waterpipe configuration on the cytotoxicity of the smoke produced. Shisha and puff topography were held constant while the height of the waterpipe was varied between 11.5, 21, and 46.5 cm, and the length and composition of the hose were varied between 94 and 184 cm and Tygon® 2375 and commercial hookah plastic-wrapped metal wire, respectively. Unlike others, our research incorporates cellular exposure at the air-liquid interface at airflows more similar to those in the alveolae and allows chemical and physical effects of smoke on the epithelial cells to be studied. L2 cells (type II pneumocytes) were seeded at 10^6 cells per Transwell filter and exposed to WTS generated from different waterpipe configurations and following a modified Beirut smoking protocol. After a 24hr recovery period with the air-liquid interface maintained, the treatments' effects were analyzed by normalizing the average value for three technical replicates against that of mock-exposed cells from the same experimental run and determining the average normalized value of separate three biological replicates. Two cell viability metrics were used, membrane permeability (CellTiter Fluor, Promega) and Neutral red dye uptake (NRU). As indicated by variances, one way ANOVA or Kruskal Wallis rank sum test statistical analyses were performed to understand the differences due to the different conditions and whether the smoke produced met the NIH definition of a toxic substance.

11HA.8

Use of Cleaning Sprays: Respiratory and Musculoskeletal Human Health Effects Studied in an Exposure Chamber.

KARIN LOVÉN, Jörn Nielsen, Eva Assarsson, Pia Tallving, Monica Kåredal, Aneta Wierzbicka, Camilla Dahlqvist, Catarina Nordander, Yiyi Xu, Anders Gudmundsson, Christina Isaxon, *Ergonomics and Aerosol Technology, Lund University, Sweden*

Cleaning workers belong to a large occupational group, which is exposed to many risk factors, including high physical workload and handling of cleaning products. Documented risks for professional cleaners include musculoskeletal disorders as well as the development of different respiratory symptoms (Unge et al., 2007; Lillienberg et al., 2013). Spray is a cleaning method with the advantage of easy use and even and precise dosage. A survey (n=225) conducted within this study confirmed that spray cleaning products are used by about 78 % of Swedish professional cleaning workers. There are some studies (e.g. Zock et al., 2007) linking the specific use of cleaning sprays to high occurrence of development of new-onset asthma as well as other respiratory symptoms. However, no human exposure-response study have been conducted until now in order to understand how the cleaning spray aerosols affect the user.

A human exposure-response study was conducted in a 21,6 m^3 stainless steel chamber with controlled temperature, relative humidity (RH) and air exchange rate (AER). 19 volunteers; 11 female cleaning workers and 8 non-cleaning worker females, participated. The chamber was furnished as a bathroom and was cleaned using three different cleaning methods (three exposures) during three different days. The cleaning methods included A: zero exposure with only microfiber cloths, B: cleaning products applied as foam, C: cleaning products applied as spray. During the exposures, the temperature was about 22 ºC, the RH 30 % and the AER 0.9 h^{-1}.

Particle concentrations and size distributions (in the size range 0.5-20 µm) were measured in the chamber using an Aerodynamic Particle Sizer (model 3321, TSI Inc., USA). A Condensation Particle Counter (model 3010, TSI Inc., USA) was used to measure the particle concentration in the size range 0.01-1 µm and a VelociCalc (model 9565-P, probe 986, TSI Inc., USA) was used to measure the total volatile organic compound (VOC) concentrations in the chamber.

Before and after each exposure day the volunteers went through biological sampling, including blood sample, nasal lavage and exhaled condensate. Spirometry, peak nasal inspiratory flow (PNIF) and tear film break up time were measured and the subjects also filled out self-assessment questionnaires. Additional measurements of the musculoskeletal load during the zero exposure (A) and the spray exposure (C) were also conducted for the 11 cleaning workers.

During spray exposure (C) a clear increase in particle concentration (0.5-20 µm) could be seen while cleaning. Concentrations during foam exposure (B) were also slightly elevated compared to the zero exposure (A). The particle concentration (0.01-1 µm) was generally low; below 500 particles/cm^3, however, slight increases during exposure C and B, was observed. A slight difference between exposure C and B was also observed in the VOC measurements with higher concentrations for exposure C.

The preliminary results from the medical assessments showed a significant decrease in the PNIF measurements during spray exposure (C) compared to the zero exposure (A). The final results from the medical analysis and the musculoskeletal measurements will be available later this spring and will give a more comprehensive answer to how the different cleaning methods affect the user. With the results from this study, we can hopefully recommend the best cleaning application method to use with regards to both the respiratory as well as the musculoskeletal system.

This work was supported by Swedish AFA Insurance.

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11IM.1

A New Chamber for Studying Aerosol Formation and Aging in Clouds. DON COLLINS, Cassandra Milan, Geoffrey Roest, Jacob Escobedo, Ariana Castillo, Kate Godfrey, *Texas A&M University*

Aqueous phase chemical reactions inside clouds can produce low volatility species that remain in the aerosol phase after the droplets evaporate. In recent years there has been considerable interest in identifying precursor species responsible for in-cloud production of secondary organic aerosol and in quantifying the rates and products of the reactions. Whereas most studies have used homogeneous solutions containing the soluble organic precursors and oxidants, it is likely that large gradients exist in actual cloud droplets because the hydroxyl radical responsible for most oxidation will not penetrate far before reacting. The Multiphase Aging and Production of Particles (MAPP) chamber was developed primarily to study aqueous formation of secondary organic aerosol in/on cloud droplets. Clouds are formed through adiabatic expansion inside a 1.2 cubic meter all-FEP Teflon cloud/reaction chamber that is suspended in a 3.5 cubic meter stainless steel vessel that can withstand full vacuum. Air is simultaneously extracted from the reaction/cloud chamber and the surrounding vacuum vessel such that a slight positive pressure is always maintained to keep the 0.05 mm thick FEP walls taut. Air cooled with a chilled water heat exchanger and/or heated with a resistive heater is circulated around the reaction/cloud chamber to maintain the walls at about the same temperature as the air inside to minimize convection, humidity gradients, and droplet evaporation. The reaction/cloud chamber rotates on a horizontal axis at about 7 rpm to minimize settling losses of the large droplets. Water soluble precursor gases such as glyoxal can either be directly injected or formed through gas phase photochemistry driven by solar simulating lamps. Monodisperse particles are injected prior to cloud formation and their growth during the experiment is used to quantify in-cloud aerosol production. Results from preliminary cloud processing experiments will be presented.

11IM.2

Estimating Secondary Organic Aerosol Yield from Size Distribution Measurements in Chamber Experiments. WEIMENG KONG, Sophia Charan, Yuanlong Huang, Huajun Mai, John Seinfeld, Richard Flagan, *California Institute of Technology*

In order to determine secondary organic aerosol (SOA) yields in chamber experiments, size distribution measurements obtained with the differential mobility analyzer must be translated from number to mass distributions. Any uncertainty in the large particle tail of the size distribution significantly impacts the SOA estimates. Size distributions are typically obtained using the scanning electrical mobility analyzer (SEMS; also known as the scanning mobility particle sizer, SMPS). Most interpretation of SEMS data is performed using the constant-voltage differential mobility analyzer (DMA) transfer function derived using a highly idealized model of the DMA. To address biases associated with the finite time response of the CPC detector, SEMS/SMPS systems are generally operated with a relatively slow voltage scan, and convoluting the DMA transfer function with an empirically fit model of the delay-time distribution introduced by the CPC. Depending upon the quality of the delay time model employed and the details of the inversion, the large-particle tail of the particle size distribution can introduce substantial uncertainty in the estimated yield. Moreover, recent derivation of the actual transfer function for the SEMS/SMPS based on detailed numerical modeling of flows, fields, and particle transport within the TSI long column DMA during voltage scanning reveals differences from that derived for the constant voltage DMA. This study reports on the integration of this SEMS/SMPS transfer function into the data inversion process for determination of SOA yields. A number of previous chamber experiments have been reanalyzed with the new transfer function as well to explore the effects on actual experimental data, as are new experiments performed under very slow scans that minimize these instrumental effects. Simulated measurements from modeled experiments demonstrate the reduction of uncertainty in the SOA yields that results from use of the proper transfer function.

11IM.3

Effects of Gas-Wall Partitioning in Tubing and Instrumentation on Gas-phase, Aerosol, and Potential Aerosol Measurements. Demetrios Pagonis, Benjamin Deming, Xiaoxi Liu, Ranajit Talukdar, James Roberts, Jordan Krechmer, Brett Palm, Joost de Gouw, Paul Ziemann, JOSE-LUIS JIMENEZ, *University of Colorado-Boulder*

Recent studies have demonstrated that organic compounds can partition from the gas phase to the walls in Teflon environmental chambers and that the process can be modeled as absorptive partitioning. We extend these studies to investigate gas–wall partitioning of organic and inorganic compounds in tubing from multiple materials, and also to the instruments (e.g. PTRMS and CIMS) used to monitor compound concentrations. These effects can result in important perturbations for measurements of gases, aerosols, and also potential aerosols (e.g. when using oxidation flow reactors).

To quantify the effects of tubing, we measure the response to step increases and decreases in analyte concentrations. By comparing the delays seen with the instrument alone with those seen with additional tubing we can separate the instrument response and tubing delay. For Teflon tubing, rapid partitioning of C_8–C_{14} 2-ketones and C_{11}–C_{16} 1-alkenes was observed for compounds with saturation concentrations (c*) in the range of 3×10^4 to 1×10^7 μg m^{-3}, causing delays in instrument response to step-function changes in the concentration of compounds being measured. These delays vary proportionally with tubing length and diameter and inversely with flow rate and c*. The gas–wall partitioning process in Teflon tubing is similar to what occurs in a gas chromatography column, and the measured delay times (analogous to retention times) are accurately described using a linear chromatography model where the walls were treated as an equivalent absorbing mass that is consistent with values determined for Teflon environmental chambers. Instrument delays can be quantified in an analgous manner, and substantial differences between instruments are found. The model predicts delays of an hour or more for semivolatile compounds measured under commonly employed conditions. Measurements of semivolatile species in the gas or aerosol phase, and or potential SOA formation (e.g. from oxidation flow reactors) can be greatly perturbed due to inlet delays, depending on the experimental setup.

All types of Teflon (PFA, FEP, PTFE) and plastic (PEEK) show absortive behavior and can be modeled similarly, with PFA showing the best performance. Teflon tubings show no humidity dependence. Other materials commonly used in aerosol experiments (stainless steel, aluminum, glass, and others) show always larger delays than Teflon, and show very strong humidity and concentration history dependence. These materials do not fit an absorptive model, and instead appear to be dominated by adsorption to a finite number of surface sites. The delays through this second group of tubing materials can be minimized using relative humidities above 20%, and are also decreased at larger gas-phase concentration due to the saturation of the surface sites.

Small inorganic molecules behave differently than organic ones in Teflon tubing, which is explained by differences in the sorption mechanisms. Best practices for different molecules and tubing types will be presented.

11IM.4

Measuring Thermodenuder Efficacy for Model Black Carbon Systems with Non-Absorbing Coatings. JAMES RADNEY, Christopher Zangmeister, *National Institute of Standards and Technology*

Thermodenuders have become a gold standard in aerosol research for trying to remove coatings from black carbon particles (BC). Thermodenuders operate, in principle, by evaporating coatings from a non-refractory BC core in a flowing air stream with the concomitant scrubbing of the evaporated material by an activated carbon matrix. These systems are heavily used for the for the determination of the native BC and/or non-volatile components' physical, chemical and optical properties. Here, we investigate the removal efficacy – defined as the ability to return the BC particles to their native (uncoated) mass and optical cross sections (extinction and absorption) – of model coatings (salts and organic liquids of varying volatility) as a function of particle size and BC mixing ratio.

11IM.5

A Novel Method for Multi-component Continuous Real-time Aerosol Monitoring Using FTIR Spectroscopy for In-vivo Studies. WEI TECK TAN, Subash Krishnan, Patrick Vanscheeuwijck, *Philip Morris International Research Laboratories Pte Ltd*

The conduct of in-vivo studies as recommended by test guidelines (e.g. TG413) from the Organization for Economic Cooperation and Development (OECD) requires the test atmosphere to be held as constant as practicable. This is non-trivial especially in cases whereby the test item are complex multi-phase and multi-constituent aerosols from tobacco products or e-liquids.

Classical methods for quantification of non-gaseous key constituents such as determination of the test atmosphere nicotine concentration typically involves sample trapping in an appropriate medium followed by off-line analysis. This is resource intensive and provides only cumulative averages over the period of sample collection. For a more immediate assessment, a real time aerosol characterization method has been developed to quantify key aerosol constituents using Fourier Transformed Infrared (FTIR) spectroscopy.

The setup for sample processing, analysis and extraction from the test atmosphere consists of: 1) A dilutor which dilutes the sample to the concentration within the quantification limits of the FTIR if required, 2) A transfer section with heated tubes to vaporize non-gaseous components of the constituents to be quantified, 3) a heated filter at the end of the heated tubes to remove residual non-gaseous components to avoid damage to the FTIR, 4) a Gasmet FTIR spectrometer and 5) A vacuum pump for pulling the sample from the test atmosphere to the FTIR.

The measured overall IR spectra of the aerosol obtained from the test atmosphere is deconvoluted and compared in real time against reference calibration spectra using proprietary software from Gasmet to quantify the concentration in µg/L for water, propylene glycol, glycerol, and nicotine concurrently. During continuous sampling from the test atmosphere, concentrations of the aforementioned constituents can be quantified simultaneously by the FTIR in approximately every < 6 seconds.

Comparative studies were conducted using aerosol from e-liquids and the IQOS smokeless product whereby nicotine results from the FTIR were found to be within ±20% of the results from validated off-line analysis methods using gas chromatography. It is demonstrated that this method allows for real time quantification of selected key constituents and that can be used as a tool to further characterize the test atmosphere. When used for test atmosphere monitoring, the data generated in real time from the FTIR allows for earlier detection of process deviations and timely interventions which therefore improves the stability of the test atmosphere.

11IM.6

Characterization of Thermal Dissociation Cavity Attenuated Phase Shift Spectroscopy (TD-CAPS) for Total Gas-Phase and Particle-Phase Alkyl Nitrates and Peroxy Nitrates Measurements. GAMZE ERIS, Masayuki Takeuchi, Ezra Wood, David Tanner, Greg Huey, Nga Lee Ng, *Georgia Institute of Technology*

Recent field studies at various ambient sites demonstrate that the contribution of organic nitrates to total submicron organic aerosols is substantial. Organic nitrates, including alkyl nitrates (AN) and peroxy nitrates (PN), are important NO_x reservoirs or sinks in the troposphere. Formation of AN and PN terminates the chain reactions of RO_x and NO_x radicals; therefore the quantification of these nitrates is critical to understanding the global and regional distributions of NO_x as well as its cycling and impact on ozone and secondary organic aerosol (SOA) production. Organic nitrates consist of structurally distinct compounds that are usually in low concentration, which makes their quantification, challenging. To measure organic nitrates, a thermal dissociation (TD) inlet is typically coupled with various NO_y detection techniques such as Chemical Ionization Mass Spectrometry (TD-CIMS), Laser Induced Fluorescence (TD-LIF), Cavity Ring-down Spectrometer (TD-CRDS) and Cavity Attenuated Phase Shift Spectroscopy (TD-CAPS). TD-CAPS is advantageous since the CAPS monitor is commercially available, easy to setup and use, and requires little maintenance. Ambient measurements by TD-CAPS have been recently conducted in a remote region. However, characterization of the instrument with regard to interference from other atmospheric constituents and limits of detection are limited. In this work, we developed a TD-CAPS instrument to measure total AN and PN in gas and particle phase. The instrument consists of two quartz tube reactors at 563 K and 473 K (enabling decomposition of AN and PN, respectively, to NO_2) and a reference channel that measures the ambient NO_2. The NO_2 concentration in each channel is measured by a CAPS monitor. Isopropyl nitrate (IPN) and peroxy acetyl nitrate (PAN) are used as representative AN and PN compounds to identify and quantify potential chemical interferences from side reactions due to presence of atmospheric constituents such as O_3, NO and NO_2. Correction factors are derived for binary reactions of these compounds over a wide range of concentrations that is representative of rural and urban ambient environments and laboratory chamber reaction conditions. Moreover, SOA is produced from oxidation of biogenic volatile organic compounds in the Georgia Tech Environmental Chamber (GTEC) facility to evaluate the performance and further improve the TD-CAPS instrument. Various oxidants, i.e., OH, NO_3 and O_3, are reacted with isoprene and monoterpenes such as α-pinene, β-pinene and limonene to produce different organic masses with different organic nitrate products in the chamber. The gas-phase and particle-phase AN and PN are measured by the addition of a Teflon filter and activated charcoal denuder to the TD-CAPS inlet, respectively. Particle-phase organic nitrates measured by TD-CAPS are compared with those measured by High-Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS). Quantitative agreement between these two methods is observed. Gas-phase and particle-phase organic nitrates measured by TD-CAPS are also compared with observations by Filter Inlet for Gases and AEROsols (FIGAERO) High-Resolution Time-of-Flight Chemical-Ionization Mass Spectrometer (HR-ToF-CIMS) . These direct measurements of gas-phase and particle-phase organic nitrates allow us to calculate their bulk partitioning coefficients, an important parameter determining SOA formation.

11IM.7

A Quantitative Method to Measure and Speciate Amines in Ambient Aerosol Samples. AMY P. SULLIVAN, Katherine Benedict, Jeffrey Collett, *Colorado State University*

Ambient reactive nitrogen is a mix of organic compounds that contain nitrogen and inorganic compounds like nitric acid, nitrate, ammonia, and ammonium. These various forms of nitrogen are found in both the aerosol and gas phases and in oxidized and reduced forms. The aerosol-phase reduced nitrogen is predominately thought to include ammonium and amines. In ambient samples the ammonium concentration is often routinely determined, but the contribution of amines is not. This has left limited information on the abundance and speciation of amines. In addition, in the traditional cation separation methods currently used to measure ammonium and other common inorganic ions there is significant overlap with amines that is not accounted for. Therefore, we have developed a method to discretely measure amines from ambient aerosol samples. It employs ion chromatography using a Dionex CS-19 column with conductivity detection and a methanesulfonic acid eluent gradient separation. This method allows for quantification of 16 different amines, including the series of methylamines and ethylamines as well as the different isomers of butylamine, along with the common inorganic cations. Here we will present the details of the method. We will assess the impact of the presence of amines on the determination of the common inorganic ions. We will also examine data from the analysis of ambient filter samples collected in Rocky Mountain National Park and from biomass burning source testing using this method. Even in the typical background conditions encountered in Rocky Mountain National Park, from analysis of daily low flowrate samples we were able to regularly measure almost all of the various quantifiable amines this technique can identify. The sum of the amines was generally about 0.02 µg/m3. It increased to 0.04 µg/m3 when the site was being impacted by biomass burning, largely due to observable increases in methylamine and dimethylamine.

11IM.8

Analysis of Solutions by Fourier Transform Infrared Spectroscopy by Electrospray Film Deposition. ANDREA ARANGIO, Christophe Delval, Giulia Ruggeri, Satoshi Takahama, *EPFL*

Fourier transform infrared (FTIR) spectroscopy is a powerful technique that has been widely applied for functional group analysis and organic matter quantification in atmospheric aerosol particles. However, FTIR transmission spectroscopy of particles collected on Teflon filters render some regions of the infrared spectrum inaccessible due to interferences from the substrate. Additionally, significant background correction of spectra is required to account for the Teflon absorption and scattering to obtain the actual spectrum of the particulate matter sampled. Transmission analysis with FTIR is not applicable for particles collected on quartz-fiber filters because of the high IR-absorption of the quartz. To overcome the filter interferences and extend FTIR applicability, solvent extraction protocols are typically applied to analyse soluble fractions of particulate matter.

FTIR analysis of filter extracts is also complicated by the significant IR-absorption of solvents but these issues can be circumvented by applying solvent-elimination techniques. In these approaches, the solvent is evaporated while the separated compounds are immobilised on a substrate prior to the collection of the FTIR spectrum.

In this work we present a rapid solvent-elimination method based on electrospray technique to isolate analytes for chemical characterization. Extracted solutions from filters are purged through an electrified needle to generate a spray in which micro-droplets allow fast solvent evaporation. The resulting solutes are deposited onto a grounded Internal Reflection Element (IRE) to apply Attenuated Total Reflectance - FTIR (ATR-FTIR) spectroscopy. ATR-FTIR is a sensitive technique with capability to analyse submicrogram quantities of analytes and is therefore selected to obtain the maximum signal-to-noise ratio. Several parameters that affect the electrospray film deposition, together with the linearity of the response over a wide mass range are investigated for volatile and non-volatile organic compounds and inorganic salts. The method is highly reproducible and the instrumental limit of detection is as low as 250 ng.

11LC.1

Residential PM Measured in 50 Homes Using Low-cost Monitors over Two Heating Seasons in Rochester, NY.

Gursumeeran Satsangi, Mauro Masiol, Nadežda Zíková, David C. Chalupa, David Q. Rich, Philip K. Hopke, ANDREA R. FERRO, *Clarkson University*

Heating appliances using wood and wood products for combustion are a major source of airborne PM and related pollutants during the heating season in Rochester, NY (Wang et al., 2012). Although most regulatory short-term PM monitoring is based on 24-h integrated measurements in relatively few locations, health outcomes may be triggered by increases in PM concentrations in the previous few hours (e.g., Gardner et al., 2014), and PM concentrations can vary greatly across an urban area (Zikova et al., 2017a). Temporally and spatially resolved estimates of PM exposure to wood smoke and other sources are needed to understand how health outcomes are associated with increases in PM concentration a few hours later.

Continuous 1-minute indoor and outdoor PM concentrations were measured from November through April of 2015/16 and 2016/17 at 25 residences per season across Monroe County, New York using Speck (Airviz Inc., Pittsburgh, PA) low-cost monitors (LCMs). Study participants either had wood burning appliances in their homes or reported that they often smelled wood smoke near their homes. CO concentration was measured in the main living area of the homes using data loggers with electrochemical sensors (EL-USB-CO, Lascar Electronics, Erie, PA). During the 2016/17 season, a thermocouple with a datalogger was attached to the wood burning appliance. The Speck LCMs were found to be reasonably precise but with a large bias (Zikova et al., 2017a,b). To correct the bias, the Speck LCM measurements were adjusted to the ratio of the average PM2.5 concentration measured by a GRIMM 1.109 aerosol spectrometer (Douglasville, GA, USA) to the average concentration for each Speck LCM during a multi-day collocation period.

The mean indoor/outdoor (I/O) PM ratio was 1.7 for all homes and increased to 2.5 when a combustion source was operated as indicated by an elevated CO concentration. Increases in wood-burning appliance temperature and indoor CO concentrations were found to be associated with an overall moderate (mean value of several $\mu g/m^3$) increase in indoor PM concentration averaged over the heating season. Short-term PM increases greater than 100 $\mu g/m^3$ were periodically observed in homes with and without wood-burning appliances operating. The concentration pattern showed clear morning and evening peaks as well as higher indoor concentrations during the weekends when people are typically at home.

The concentrations measured by the LCMs at 25 homes were often lower than the estimated limit of detection of 10 $\mu g/m^3$, and the outdoor bias-corrected LCM measurements were ~40% of the mean PM2.5 concentrations measured by the FEM located within the study geographic area (Zikova et al., 2017a,b). Also, many combustion particles are in the size range below the nominal 0.5 µm sensor lower limit of detection. Thus, the PM concentrations produced by combustion sources are likely to have been underestimated in this study.

This study provides an approach for exposure assessment in individual homes that can be utilized by employing appropriate calibration and quality assurance procedures for the LCMs.

Acknowledgement
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11LC.2

Results from the Citizen-Enabled Aerosol Measurements for Satellites (CEAMS) Pilot Campaign in Northern Colorado.

Bonne Ford, Jeffrey R. Pierce, Eric Wendt, Marilee Long, Shantanu Jathar, Jessica Tryner, Casey Quinn, Lizette Van Zyl, John Mehaffy, Christian L'Orange, Dan Miller-Lionberg, JOHN VOLCKENS, *Colorado State University*

Atmospheric particulate matter with diameter smaller than 2.5 µm ($PM_{2.5}$) is a pollutant that contributes to the development of human disease. Routine monitoring of ground-level concentrations generally relies on instruments which are often prohibitively expensive for mass deployment across the globe. However, satellite-derived estimates of surface-level $PM_{2.5}$ have the potential to provide information on the global $PM_{2.5}$ distribution. These estimates rely on information about the ratio of $PM_{2.5}$ to AOD (aerosol optical depth, primary aerosol retrieval made by satellites), of which there are few co-located measurements for validation.

In this project, we demonstrated the capability of training citizen scientists to use low-cost, high-quality samplers that simultaneously measure AOD and $PM_{2.5}$ (integrated filter and real-time sensor) to collect daily $PM_{2.5}$:AOD ratios over northern Colorado for several seasons in 2017 and 2018. This presentation will discuss our pilot citizen-science campaign, including recruitment and training findings, along with our $PM_{2.5}$:AOD ratio dataset. A project website, social media accounts, and training materials were developed. A panel of 30 citizen scientists were recruited to participate in the CEAMS (Citizen-Enabled Aerosol Measurements for Satellites) pilot deployment. Following a series of trainings, more than 150 successful instantaneous AOD measurements and 50 $PM_{2.5}$ filters (48-hour averages) were collected by the citizen scientists, with relatively high compliance and good agreement between measurements.

By training citizen scientists to take measurements in their backyards, we were able to create an extensive network with high spatial density that provides insight into local air quality distributions. Data from our citizen-science network demonstrated substantial variability in measured $PM_{2.5}$:AOD ratios within a single 10x10 km grid (more than can be explained by measurement error alone); these results demonstrate the need for more spatially and temporally resolved measurements of this ratio to improve satellite-derived estimates. Another impactful product from this citizen-science network was the discovery of residential woodsmoke impacts in the “Old Town” region of Fort Collins, CO. This region, which features a high density of older homes with working fireplaces, demonstrated substantial increases in $PM_{2.5}$ concentrations during wintertime nights.

11LC.3

Prevalence and Timing of Indoor PM Emission Events Observed in a Small Cohort of Homes Using Low-Cost Dust Sensors.

Ian Longley, Gustavo Olivares, Ayushi Kachhara, Sam Edwards, GUY COULSON, *National Inst of Water and Atmospheric Research, New Zealand*

Home occupants are exposed to airborne particulate matter from both indoor sources and the infiltration of outdoor sources. Mostly this differentiation has been achieved through compositional analysis. We conducted a pilot study using time series analysis of continuous data from a low-cost unobtrusive sensor package that would be suitable for mass deployment.

Eight homes were equipped with three custom-built air quality monitors for a 2-week period in winter 2016. Two monitors (PACMAN) were placed in two rooms indoors and one (ODIN) outdoors on the same property. All homes but one used wood-burning appliances as the primary source of heat and were all located in a town where wood-burning dominates both heating and PM emissions. Householders were invited to keep time-activity diaries focusing on cooking, heating and other activities which may impact PM levels in the home, and fire-lighting was monitored with temperature sensors.

Distinct particle ‘events’ were detectable in every home in which PM levels rapidly increased then decayed. Events were attributed to indoor or outdoor sources depending on whether a corresponding event was observed outdoors or not. The average prevalence of indoor sources was 1.2 per day (range 0.8 – 1.5). Events were attributed to outdoor sources in 6 out of 8 houses with an average prevalence of 0.4 events per day. Indoor events produced peak concentrations 3 times greater than outdoor events on average. Indoor source events were most common between 7 am and 8 am and between 5 pm and 6 pm, but with variations between homes. Outdoor source events appeared to have no temporal pattern. Completion of time-activity diaries, and the detail provided was highly variable. However, there was no clear correlation between events described and observed particle levels. Particle events did not, in general, correspond to the lighting of wood-burning fires. Data was visualised for presentation to, and discussion with, householders.

11LC.4

Low-cost Sensing of Aerosol Active Surface Area by Direct Ultraviolet Photoionization. ROBERT NISHIDA, Tyler J. Johnson, Adam M Boies, John Saffell, Simone Hochgreb, *University of Cambridge*

Direct ultraviolet (UV) photoemission yields electrical current measurements proportional to aerosol active surface area which is of interest for emissions and environmental monitoring. We have demonstrated a low-cost, proof-of-concept device for using UV photoionization and detection electronics to yield direct, real-time total active surface area measurements of some ultrafine particle materials (Nishida, Boies, & Hochgreb, 2018). However, the fundamental mechanisms of photoemission must be understood to accurately interpret measurements in the field.

The particle mobility diameter may be used to describe an active particle surface which interacts with gas molecules producing a drag force for both spheres and agglomerates. Photoionization measurements yield signals proportional to the active surface, however, for the same aerosol material, previous research has found a morphology dependency distinct from mobility diameter which disagrees with existing photocharging theory (Keller, Fierz, Siegmann, Siegmann, & Filippov, 2001; Zhou, You, Tan, & Zachariah, 2013). This work aims to isolate the effect of particle morphology in order to improve photoelectric charging theory for accurate interpretation of in-field measurements.

In this work, photoemission theory is evaluated by analysing photoelectric current measurements for a range of aerosol particle types, sizes, concentrations, and morphologies. Neutrally charged, sintered silver spheres and aggregates are classified with an aerodynamic aerosol classifier (AAC) and subsequently measured with a scanning mobility particle sizer (SMPS) and photoionization sensor in parallel. This configuration allows a direct comparison of aerosols of the same material and electrical mobility, but with different morphologies. Results confirm that total photoelectric yield of both silver aggregates and spheres is a linear function of active surface area, however, it is found that silver aggregates exhibit a higher photoelectric yield than spheres of the same mobility diameter in contrast with previous research. Photoemission measurements from raw and thermo-denuded flame soot confirm surface-dependent effects on photoemission yield.

Photoemission theory is evaluated for the applicability of its experimental constants, including a single empirical constant and a particle work function for each material to account for photoionization. Results suggest photoelectric charging theory should include a morphology dependency. The method of detecting particle size and concentration parameters is evaluated in terms of experimental uncertainty and applicability in a commercial low-cost, environmental monitoring device for ultrafines.

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11LC.5

Mapping Occupational Hazards with a Multi-Hazard Monitor Network in a Heavy-Vehicle Manufacturing Facility.

CHRISTOPHER ZUIDEMA, Sinan Sousan, Nima Afshar-Mohajer, Larissa Stebounova, Alyson Gray, Laura Hallett, Xiaoxing Liu, Marcus Tatum, Mitch Fitzpatrick, Oliver Stroh, Campbell Summer, Geb Thomas, Thomas Peters, Kirsten Koehler,
Johns Hopkins School of Public Health

Sensors play an important role in the lower-accuracy/ larger sample measurement paradigm emerging in environmental health. Due to their small size, low power demands and interoperability, low-cost sensors can be deployed in collections that are spatially distributed in the environment, known as sensor or monitor networks. Although examples of these networks in the ambient environment exist in the literature, we have developed and deployed 40 multi-hazard monitors, constructed with low-cost sensors for particulate matter (SHARP GP), carbon monoxide (Alphasense CO-B4), oxidative gases (Alphasense OX-B431) and noise (developed in-house) in a wireless network in a heavy-vehicle manufacturing facility. Monitors were equipped with radio antennae that communicated with a central database and recorded hazard measurements at 5-minute intervals. Here, we report on the temporospatial measurements from the monitor network, precision of network measurements, and accuracy of network measurements with respect to field reference instruments after approximately 5 months of continuous deployment. During 'first shift' production periods, 1-hr mean hazard levels across all monitors for PM, CO, oxidative gases and noise ranged from 0.4-0.6 mg/m^3, 2-10 ppm, 50-150 ppb, and 78-83 dBA respectively. We examined the influence of major manufacturing processes on the spatial variability of hazards by grouping monitors by the processes that surrounded them. Manufacturing processes associated with the highest hazard levels were flame cutting (PM), staging (CO), machining (oxidative gases) and machining and welding (noise). We observed clear diurnal and weekly temporal patterns in the mean level of each hazard, and daily, hazard-specific spatial patterns attributable to general manufacturing processes in the facility, for example welding, machining and laser cutting. Monitors exhibited varying degrees of measurement precision across the range of hazard levels observed, and the maximum difference between 3 collocated monitors and their mean was equal to 0.4 mg/m^3 for PM, 2.5 ppm for CO, 25 ppb for oxidative gases, and 2 dBA for noise. The second-order coefficient of variation (V_2) for 3 collocated monitors was equal to 0.17, 0.02, 0.02, and 0.00, for PM, CO, oxidative gases and noise, respectively, at the median hazard level observed. We assessed the accuracy of monitors in the network by conducting side-by-side measurements with field reference instruments and observed the median percent bias for each hazard equal to -17.8%, -0.9%, -25% and 0.3%, for PM, CO, oxidative gases and noise respectively. This study demonstrates the long-term deployment of a multi-hazard monitor network in an industrial manufacturing setting, advances techniques to comprehensively map occupational hazards and sets the stage for using monitor networks to characterize occupational exposures on the individual level.

11LC.6

Low-Cost Particle Sensor for Monitoring Real-Time Protection of Respirators. BINGBING WU, Maija Leppänen, Jonathan Corey, Michael Yermakov, Yan Liu, Sergey A. Grinshpun, *University of Cincinnati*

Elastomeric particulate half- and full-facepiece respirators equipped with HEPA filters generally provide a high level of protection against various aerosol particles. Penetration of relatively large particles (approximately 0.5 µm and above) through a typical HEPA filter is extraordinarily low and usually undetectable. If these large particles penetrate an elastomeric respirator in any significant quantity, one could reasonably expect that this occurred due to a failure in respirator fit. Respators are prone to faceseal leakage, which often represents the primary penetration pathway. Therefore, it would be useful to monitor the aerosol concentration inside the respirator during work activities with a portable sensor capable of detecting relatively large aerosol particles in real time. If detected, one may conclude that the face seal integrity is compromised. Recent developments in aerosol instrumentation have led to low-cost, ultra-small optical particle sensors. In this study, a low-cost, portable Respirator Seal Integrity Monitor (ReSIM) was developed and evaluated.

The ReSIM prototype is based on a low-cost optical particle sensor (PPD60PV-T2, Shinyei, Kobe, Japan). It is designed to perform continuous air sampling inside a respirator, process all particle detection events over every 30-second interval and identify sudden particle concentration increases corresponding to faceseal leakage.
ReSIM was first evaluated using a respirator-wearing manikin set-up and thereafter tested with firefighters engaging in simulated workplace activities in a 24.3-m^3 laboratory exposure chamber. Two challenges, NaCl aerosol and combustion aerosol, were generated in the chamber during the manikin study. Only NaCl aerosol was generated when testing ReSIM on human subjects (firefighters). The tests in the manikin-based set-up were performed at three breathing flow rates: 30, 60 and 85 L/min.

While ReSIM performed in-mask air sampling from the respirator donned either on a manikin or on a subject, an operator intermediately induced leaks using a solenoid control valve and closed the valve to maintain a tight faceseal. Additional leaks were established by each human subject slightly repositioning the respirator on his/her faces, which commonly occurs in practice. A reference optical aerosol spectrometer (OAS, Model 1.108, Grimm Technologies) was connected to the same sampling probe as ReSIM. Its role was to confirm that a faceseal leakage was successfully established. It also verified that no large particles (within the optical range) penetrated while the respirator was fully sealed.

The leak detection performance of ReSIM was evaluated in terms of sensitivity and specificity. Sensitivity is defined as the probability of correct identification of the intervals with leaks, whereas specificity refers to the probability of correct identification of the intervals with no leaks.

When tested on the manikin, the ReSIM provided leak detection sensitivities of 71.8% and 98.4% when challenged with NaCl and combustion aerosol, respectively. The specificity was 99.8% for both aerosols. A lower sensitivity (58.0%) was obtained when testing with human subjects and NaCl; however, it should be higher for combustion aerosols based on the manikin-based study findings. When tested on firefighters, ReSIM demonstrated a specificity of 96.1%. Lower sensitivity and specificity values obtained with subjects compared to the manikin-generated data could be primarily attributed to the effect of moisture on the particle sensor, variability among subjects, and in-mask sampling bias.

In summary, ReSIM demonstrated its ability to assess the real-time respirator performance during actual use with sufficient sensitivity and rather high specificity. With an integrated alarm system, this response would trigger an alarm signaling the wearer that he/she can be overexposed to aerosol hazards.

11LC.7

Deployment of Low-cost Sensors to Assess the Impacts of Portable Air Filtration on Indoor PM2.5 and Associated Personal Exposure. KAROLINE JOHNSON, Christina Norris, Tongshu Zheng, Michael Bergin, James Schauer, Junfeng Zhang, Yinping Zhang, *Duke University*

In highly polluted Chinese cities, air purifiers are used in an attempt to reduce exposure to air pollution. The impacts of air purifiers on indoor air quality, personal exposure, and the resulting health impacts can differ greatly depending on a number of factors including the purifier selected, participant behavior patterns, home design, and indoor sources of pollutants. During this study, forty-three asthmatic children were recruited from around suburban Shanghai. Portable air filtration devices were installed in the children's bedrooms and operated as true purifiers for 2 weeks and as sham purifiers (without the filter media installed) for 2 weeks. During the project, participants were instructed to keep the windows and doors in the room closed. Air quality sensor packages were installed in each child's bedroom, and outside ~50% of the homes. Sensor packages contained Plantower sensors for fine particulate matter ($PM_{2.5}$) and Alphasense sensors for ozone (O_3). About 80% of the child participants carried a personal monitoring bag for a 48-hour period during both true and sham filtration. Air quality and health monitoring occurred from February until April of 2017. Ambient $PM_{2.5}$ and O_3 concentrations from a nearby monitoring site varied over this 3-month time period with concentrations averaging 56 $\mu g\ m^{-3}$ for $PM_{2.5}$ and 81 ppb for O_3. Since ambient pollutant concentrations varied over the project and indoor concentration and personal exposure are typically a function of outdoor concentration, purifier performance has been evaluated by comparing indoor to outdoor (I/O) ratios and personal to outdoor ratios during true and sham filtration. Preliminary results show average $PM_{2.5}$ indoor to outdoor ratios below 1 during sham filtration (I/O = 0.6) and lower ratios during true filtration (I/O = 0.2). Purifiers appear to have lowered indoor to outdoor $PM_{2.5}$ ratios by roughly 70%. Forty homes had successful indoor monitoring and all but two homes saw reductions of indoor to outdoor ratios of >30%. Reductions in $PM_{2.5}$ personal exposure to outdoor ratios decreased by roughly 30% on average. Further analyses highlight the microenvironments that were the highest contributors to personal exposure. The purifiers do not appear to reduce indoor O_3. The results of this project provide important information on the impacts of portable air filtration on children's exposure in China.

11LC.8

Air Quality Monitoring in the San Juan Metro Area in the Aftermath of Hurricane Maria Using Lower-Cost RAMP Monitors. ELVIS TORRES-DELGADO, R. Subramanian, Aja Ellis, Carl Malings, Rebecca Tanzer, Maité Morales-Medina, Felipe Rivera-Adorno, Darrel Baumgardner, Albert Presto, Stephan Borrmann, Roberto Rondanelli, Mirko Del Hoyo, Rémi Losno, Olga L. Mayol-Bracero, *University of Puerto Rico*

In the aftermath of Hurricane Maria, the electricity grid in Puerto Rico was devastated, with over 90% of the island without electricity. While the electricity grid is being repaired, backup generators are widely used, sometimes as the main source of electricity. The hurricane also damaged the island's existing air monitoring network and the University of Puerto Rico's (UPR) observing facilities. We deployed four lower-cost air quality monitors (Real-time Affordable Multi-Pollutant sensors, RAMPs), a Met-One black carbon (BC) monitor, and an Aeth Labs micro Aethalometer in the San Juan Metro Area in November 2017. Later, we installed an Optical Particle Counter (OPC) and a condensation Particle Counter (CPC). The first month of data collected with the RAMPs shows high sulfur dioxide (SO2) and carbon monoxide (CO) concentrations of varying magnitudes each night. SO2 and CO were strongly correlated (r2 >0.9) with each other at two locations ~5 km apart (UPR and an industrial area, Puerto Nuevo), suggesting a single source type. BC measured at the UPR site is also well correlated with CO and SO2. While the RAMPs are not certified as a federal equivalent method, the RAMP SO2 data suggests that the EPA's daily 1-hour maximum standard for SO2 (75 ppb) was exceeded on almost 80% of the first 30 days of deployment. In the wake of Hurricane Maria, Puerto Rico was granted a waiver from ultralow sulfur diesel (ULSD) requirements which, coupled with the continuing lack of grid power, appears to have significantly degraded the air quality in the region. In this presentation, we will show results from nine months of sampling at different locations across the San Juan Metro Area, including the effects of electricity grid restoration as the rebuilding work progresses.

11MG.1

Quantification of the Rapid Photochemical Secondary Organic Aerosol Production Observed across Megacities around the World. BENJAMIN A. NAULT, Pedro Campuzano-Jost, Douglas Day, Jason Schroder, Donald Blake, Manjula Canagaratna, Joost de Gouw, Jessica Gilman, Tom Hanisco, Greg Huey, B. Thomas Jobson, Bill Kuster, Barry Lefer, Jin Liao, Ilana Pollack, Jeff Peischl, James Roberts, Thomas Ryerson, Alan Fried, Bernhard Rappenglueck, Jochen Stutz, Petter Weibring, Frank Flocke, Jose-Luis Jimenez, et al., *University of Colorado-Boulder*

Organic aerosol (OA) is an important fraction of the submicron aerosol budget over urban areas around the world, with substantial and rapid secondary OA (SOA) production observed in all megacities studied to date. However, multiple studies over different megacities have shown that SOA formation cannot be accounted for when only considering traditional volatile precursor compounds (e.g., aromatics). Either other sources of SOA, including semi-volatile and intermediate-volatility anthropogenic volatile compounds (S/IVOCs) and glyoxal uptake, or much higher SOA yields for the VOC precursors are needed to account for the observed urban SOA production. Models including S/IVOCs have shown the most success in capturing the SOA production in megacities.

Using data from major megacities (Houston, 2000 and 2013, Mexico City, Los Angeles, Beijing, and Seoul) around the world, we further explore the photochemical aspects and the importance of S/IVOCs to urban SOA production. With these data, we find differences in the emission normalized SOA production for these cities that are remarkably consistent with differences in the slopes of SOA versus various other secondary photochemical species (ozone, formaldehyde, and peroxy acyl nitrate). We found that these can be explained by the differences in the mixtures of hydrocarbons emitted in the different cities. In megacities, when aromatics are more important, the hydrocarbon mixture is more efficient, per OH molecule reacted, in producing SOA, relative to the gas-phase photochemical products; whereas, when small alkenes are more important, the opposite is true. We show that this relationship has a very strong linear relationship across megacities around the world. We also discuss how the slopes between OOA and secondary photochemical species not only demonstrate that photochemical production of SOA dominates the OA budget over megacities, but how these slopes provide insight into the effective SOA yield from the hydrocarbon emissions in an urban area. The effective SOA yields from these slopes further suggest the importance of S/IVOCs to explain the observed SOA over megacities. The results from this study will allow improved quantification of urban SOA production and more accurate predictions in chemical transport models.

11MG.2

New Insights into Sources of Organic Aerosol in PM2.5 in a Polluted Urban Environment. YAN ZHENG, Qi Chen, Yaowei Li, Xi Cheng, Ying Liu, Tong Zhu, John Jayne, Douglas Worsnop, *Peking University*

Air pollution caused by fine particles is of great concern in megacities because of its significant effects on visibility, radiation, and human health. In recent years, on-line instruments like Aerodyne aerosol mass spectrometer and aerosol chemical speciation monitor are commonly used to characterize the aerosol composition and the sources of organic aerosol (OA) in China. Most of these instruments can only detect the submicron domain. However, particles having diameters of 1 to 2.5 µm may have significant contributions to the mass of fine particles in the urban environment. In this study, we deployed a time-of-flight aerosol chemical speciation monitor equipped with the 2.5-µm aerodynamic lens, a capture vaporizer, and a novel sampling-size auto-switching system in Beijing during 2016 to 2017. Non-refractory submicron and fine particles were alternatively detected for every half an hour by the same mass spectrometer, which allows source apportionments of OA in two size domains without complications from instrument differences. Submicron particles usually contribute to the majority of fine-particle mass. During the haze events, the ratio of submicron- to fine-mode non-refractory particle mass can decrease to about 0.5. The mass fractions of chemical components are similar for submicron and fine particles, although in some cases, the fractions differ in the two size domains. In summer, the sources of OA identified by positive matrix factorization are different for submicron and fine size domains. Four factors such as hydrocarbon-like OA, cooking OA, and two types of oxidized OA were resolved for submicron particles, which is consistent with the findings of previous studies. Besides, two other types of OA factors are identified for fine particles, suggesting underrepresented OA sources by previous studies.

11MG.3

Brown Carbon Aerosol in Urban Xi'an, Northwest China: The Composition and Light Absorption Properties. RUJIN HUANG, Lu Yang, Junji Cao, *Institute of Earth and Envir., Chinese Academy of Sciences*

Light-absorbing organic carbon (i.e., brown carbon or BrC) in the atmospheric aerosol has significant contribution to light absorption and radiative forcing. However, the link between BrC optical properties and chemical composition remains poorly constrained. In this study, we combine spectrophotometric measurements and chemical analyses of BrC samples collected from July 2008 to June 2009 in urban Xi'an, Northwest China. Elevated BrC was observed in winter (5 times higher than summer), largely due to increased emissions from wintertime domestic biomass burning. The light absorption coefficient of methanol-soluble BrC at 365 nm (on average approximately twice that of water-soluble BrC) was found to correlate strongly with both parent polycyclic aromatic hydrocarbons (parent-PAHs, 27 species) and their carbonyl oxygenated derivatives (carbonyl-OPAHs, 15 species) in all seasons (r^2 >0.61). These measured parent-PAHs and carbonyl-OPAHs account for on average ~1.7% of the overall absorption of methanol-soluble BrC, about 5 times higher than their mass fraction in total organic carbon (OC, ~0.35%). The fractional solar absorption by BrC relative to element carbon (EC) in the ultraviolet range (300-400 nm) is significant during winter (42±18% for water-soluble BrC and 76±29% for methanol-soluble BrC), which may greatly affect the radiative balance and tropospheric photochemistry and therefore the climate and air quality.

11MG.4

A Comparison between Satellite Observations and Ground Measurements for Fine Particulate Matter in Karachi, Pakistan.

Zhuldyz Darynova, MEHDI AMOUEI TORKMAHALLEH, Haider Khwaja, *Chemical and Aerosol Research Team, Nazarbayev University*

Karachi (total population of 18 million) in Pakistan experiences desert areas with insufficient rainfall. It also experiences humid climate in the summer and dry in the winter. The average monthly temperature varies from 13oC to 34oC. In April and August, the temperatures are high, ranging between 30 and 44oC. Several industries present in Karachi including oil-fired power plants, cement factories, steel mills, scrap metal recycling plants, shipping, railroad yards, foundries, jute and textiles, oil refineries, heavy petrochemical industries, automobile assembly plants, pharmaceuticals, printing and publishing plants, food processing plants, paper mills, chemical, glass and ceramics, battery, tanneries, brick kilns, and several light industries. A solid waste incineration plant where open burning of municipal wastes takes place is also in this city.

Ground monitoring of air pollution was conducted for a period of 12 months (August 2008 to August 2009) for PM2.5 at two individual stations at Korangi (industrial/residential) and Tibet Center (commercial/residential), located on M.A. Jinnah road in Saddar town. The M.A. Jinnah road is located in the middle of a large central business district and is the busiest road throughout the day. About 300,000 vehicles pass M. A. Jinnah road everyday. The Korangi industrial area is known as the second largest industrial area of Karachi. Around 2000 industries of different types are located in this area, including refineries, textile, chemical, and tanneries (.100 units). Sampling duration in this study was 24h (7:00 a.m to 7:00 a.m) at each place for 6 weeks in each quarter (i.e., January–March; April–June; July–September; and October–December). In our study we will also develop several statistical models to utilize satellite based measurements and evaluate capability of this method in predicting PM2.5 concentrations over the atmosphere of Karachi. Specifically, the Moderate Resolution Imaging Spectrodiometer (MODIS), instrument on board of the satellite Terra and Aqua from the NASA allows us to estimate ground-level PM2.5. It is achieved by determining Aerosol Optical Depth (AOD) which reflects optical characteristics of aerosols. The mean ground PM2.5 concentrations in Korangi and Tibet Center during winter time were found to be 111.6 and 104.3 µg/m3, respectively. However, these values were 87.5 and 73.2, in the summer, respectively. The daily measured PM2.5 concentration in 2008 and 2009 will be compared with the satellite data to find the potential correlations between satellite and the ground measurements for future studies in Karachi.

11MG.5

Chemical and Optical Characteristics of PM2.5 at an Urban Site in Gwangju during Spring 2016. JIHYO CHONG, Kwangyul Lee, Tsatsral Batmunkh, Hee-Joo Cho, Hungsoo Joo, Min-Suk Bae, Kihong Park, *Gwangju Institute of Science and Technology*

Integrated aerosol ($PM_{2.5}$) measurements such as mass concentration and chemical compositions together with the aerosol optical properties were conducted at an urban site of Gwanjgu from March to April, 2016. Filter samples were collected daily to determine the water-soluble inorganic ions (sulfate, nitrate, chloride, ammonium, sodium, potassium, calcium and magnesium), organic carbon (OC) and elemental carbon (EC) in $PM_{2.5}$. OC and EC concentrations were measured using a Sunset OC/EC analyzer (model 3F; Sunset Laboratory Inc., Tigard, OR, USA). The mass concentration of PM2.5 ranged from 0.40 to 129.40 µg/m^3 with the average value of 29.88±20.19 µg/m^3. The major ions were NO_3^-, SO_4^{2-} and NH_4^+, contributing 40.0%, 31.8% and 22.6% to the total $PM_{2.5}$ mass. The high NO_3^-/SO_4^{2-} ratio suggested that vehicular exhaust made an important contribution to atmospheric pollution. Average OC and EC concentrations were 7.33 µgC/m^3 and 0.87 µgC/m^3, taking possession of 18.4% and 2.2% of the $PM_{2.5}$ mass, respectively. In addition, the black carbon (BC) and total mass concentrations of particulate matter less than 2.5 µm ($PM_{2.5}$) were measured at Gwangju Institute of Science and Technology (GIST) measurement site to examine the relationship between the chemical compositions and optical characteristics of particles. Particulate matter (PM) events were defined depending on the mass concentration of PM (< 2.5 µm), air mass backward-trajectory, that was calculated using the Hybrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) model (Draxler and Rolph, 2013). In addition, aerosol optical properties including aerosol optical depth (AOD) were measured using a sunphotometer (Holben et al., 1998) and AODs were retrieved from MODIS Terra satellite products (Li et al., 2007; Ruiz-Arias et al., 2013).

11MG.6

Particle Concentration and Particle Size Distribution in an Urban and an Agricultural Sites in Colombia. LADY MATEUS, Angela Vargas, Jennifer Marin, Nestor Rojas, German Ruega, Rodrigo Jimenez, *Universidad Nacional de Colombia*

Particulate matter is the main air pollutant in most of the sites with air quality monitoring in Colombia. Urban PM pollution was associated with more than 10,000 premature death cases and 68 million reported symptoms and hospital visits in 2015, accounting for 1.93% of the National GDP. Despite its importance, PM has not been well characterized. Chemical speciation has been scarce, for a few source apportionment studies, and particle size distribution has been measured only in a couple of studies.

In this study, we measured Particle Concentrations (PC) and Particle Number Size Distributions (PNSD) at two sites with significantly different features. The first 2 sites were located in air quality monitoring stations in Bogota, a city with 8 million inhabitants and nearly 2-million vehicles and motorcycles, considered as one of the most densely populated cities in Latin America. One of the sites was in an urban-background area and the other was affected by traffic and industrial emissions. The third site was located on a building rooftop at the National University campus in Palmira, a city with 350,000 inhabitants in the Cauca river Valley in southwestern Colombia, the center of the sugar cane agroindustry in the country. Pre-harvest burning occurs frequently around Palmira, emitting significant amounts or PM.

We used an Electrical Low-Pressure Impactor – ELPI+ (Dekati, Finland) to examine weekly and diurnal cycles of PC and changes in PNSD that show the influence of different sources and atmospheric effects. Preliminary results show that PC in Bogota's urban background are between 3,637 and 23,040, with an arithmetic average of 10,910, with peaks during traffic rush hours. In Palmira, PC ranges between 7,809 and 35,837, with an arithmetic average of 20,903, with peaks at different times, mostly between 5 and 10 a.m. and between 8 p.m. and 3 a.m. at night. The PNSD are very dynamic in Palmira and Bogota, the small particles with an aerodynamic diameter between 10 and 100 nm increase at night until 60000 and 12000 particles/cm3, respectively.

11MG.7

Atmospheric New Particle Formation from Sulfuric Acid and Amines in a Chinese Megacity. Lei Yao, Olga Garmash, Federico Bianchi, Jun Zheng, Chao Yan, Jenni Kontkanen, Heikki Junninen, Stephany Mazon, Mikael Ehn, Pauli Paasonen, Mikko Sipilä, Mingyi Wang, Xinke Wang, Shan Xiao, Hangfei Chen, Yiqun Lu, Bowen Zhang, Dongfang Wang, QingYan Fu, Fuhai Geng, Li Li, Hongli Wang, Liping Qiao, LIN WANG, et al., *Fudan University*

Atmospheric new particle formation (NPF) is a global and important phenomenon that is yet extremely sensitive to ambient conditions. According to both observation and theoretical arguments, NPF usually requires a relatively high H2SO4 concentration to promote the formation of new particles and a low pre-existing aerosol loading to minimize the sink of new particles. However, recent observations of NPF in heavily-polluted megacities, despite enormous aerosol loadings that correspond to a large condensation sink, contradict previous knowledge that newly-formed molecular clusters should be efficiently scavenged before they reach sizes of a few nanometers, making it one of the least understood topics in atmospheric chemistry. Here, we investigated NPF in Shanghai and were able to observe both precursor vapors (H2SO4) and initial clusters at a molecular level in a megacity. High new particle formation rates were observed to coincide with several familiar markers suggestive of H2SO4-dimethylamine (DMA)-H2O nucleation, including sulfuric acid dimers and H2SO4-DMA clusters. The initial growth up to around 3 nm could be explained qualitatively by H2SO4 and neutralizing bases under the very high urban condensation sink, whereas the subsequent faster growth rate above this size is believed to result from the added contribution of condensing organic species. These findings will help to understand urban NPF and its air quality and climate impact as well as to formulate policies to mitigate secondary particle formation in China.

11MG.8

Submicron Aerosol at a Receptor Site in New Delhi: Interpreting Sources and Their Origin. SAHIL BHANDARI, Shahzad Gani, Dongyu S. Wang, Kanan Patel, Sarah Seraj, Prashant Soni, Zainab Arub, Gazala Habib, Joshua Apte, Lea Hildebrandt Ruiz, *University of Texas at Austin*

Delhi, India is the second most populous agglomeration in the world. High annual average PM_1 concentrations of about 50 µg m^{-3} and frequent severe pollution episodes, particularly in winters with concentrations as high as 500 µg m^{-3}, contribute significantly to acute and chronic PM exposure. As a part of the Delhi Aerosol Supersite (DAS) campaign, speciated submicron measurements at 1 minute time resolution have been collected from January 2017 to present at the Indian Institute of Technology Delhi using an Aerodyne Aerosol Chemical Speciation Monitor (ACSM) and an Aethalometer. Here we report the results of detailed source apportionment analysis conducted on 1.5 years of ACSM mass spectral data using positive matrix factorization (PMF). For non-refractory organics, oxidized organic aerosol (OOA) is the most important factor, contributing about 50% in all seasons. A combined organic-inorganic mass spectral (MS) PMF analyses attributes chloride almost completely to ammonium chloride. This ammonium chloride factor concentrations drop systematically from winter to summer, consistent with its volatile nature. BBOA factors indicate multiple biomass burning events that have been captured during the course of the campaign. Several episodic events associated with substantially higher concentrations compared to seasonal averages, including winter chloride concentrations of about 150 µg m^{-3} have also been detected. Heavy rainfall and monsoon events are associated with a large drop in hydrocarbon-like organic aerosol (HOA) and OOA concentrations and a complete absence of BBOA. PMF results show that OOA time series correlated well with nitrate (NO_3^-) and sulfate (SO_4^{2-}), and that HOA time series correlated well with concentrations of carbon monoxide (CO) and nitrogen oxides (NO_x) from nearby monitoring stations. We compare our PMF apportionment of BC to simpler fossil fuel and biomass burning source apportionment techniques relying strictly on Aethalometer measurements of wavelength-dependent light absorption, such as the Sandradewi et al (2008) model. Back trajectory analyses in HYSPLIT have been combined with factor and species concentrations to generate probability distribution contribution function (PSCF) and conditional probability function (CPF) rose plots identifying the local and regional nature of respective sources. These source apportionment results for Delhi can help in the development of targeted policy actions for reducing fine PM concentrations in this polluted megacity.

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12AC.1

Distribution of Organic Aerosols (OA) during the NASA ATmospheric Tomography (ATom) Campaigns: Chemical Removal and Aging as a Function of Photochemical Age. JOSE-LUIS JIMENEZ, Pedro Campuzano-Jost, Benjamin A. Nault, Jason Schroder, Douglas Day, Joseph Katich, Joshua P. Schwarz, Nicola Blake, Donald Blake, Bruce Daube, Roisin Commane, Steven Wofsy, Eric Ray, Katherine Travis, Colette Heald, Simone Tilmes, Alma Hodzic, Huisheng Bian, Peter Colarco, Mian Chin, Anna Hodshire, Jack Kodros, Jeffrey R. Pierce, *University of Colorado-Boulder*

Submicron aerosol mass in the remote free troposphere (FT) originates mostly from long-range transport from distant biogenic, anthropogenic, and biomass burning sources. Very limited local mass production in this region increases the sensitivity of aerosol concentrations to slow removal processes. As yet, few studies with an advanced aerosol payload have targeted the remote FT. Current global models exhibit a very large diversity in predicting aerosol concentrations in these regions of the atmosphere, particularly when trying to model organic aerosol (OA), which, together with sulfate, is the most prevalent type of submicron aerosols in the remote FT.

As part of NASA's Atmospheric Tomography (ATom) aircraft mission, we have acquired a global dataset of organic aerosol (OA) concentration and composition over the remote Atlantic and Pacific Oceans from 0 to 12 km and from 65 S to 80 N during four deployments encompassing the seasonal cycle for both hemispheres. This dataset provides unique new constraints on the spatial distribution of OA and its contribution to the global aerosol background; of particular interest are the OA/Sulfate ratio and OA oxidation state that are critical for estimating the activity of cloud condensation nuclei (CCN) in the remote troposphere. We find that, except for the cleanest of the ATom-sampled airmasses (less than 0.25 ug sm^{-3}), OA concentrations are comparable and often larger than sulfate.

OA was highly oxidized, significantly more than over the continental FT, with O:C ratios often in excess of 1. This translates into average OA/OC ratios in excess of 2.5, about 80% larger than what is assumed in most global OA models (1.4). Incorporating this correction into current models, as well as more accurate, revised SOA parametrizations leads to a large overprediction of OA in the FT for most models evaluated, suggesting that additional constrains on the OA lifetime in these models is needed.

Using several different hydrocarbon-ratio based photochemical clocks in combination with back-trajectories to infer the age of the airmasses sampled during ATom, we estimate that the lifetime of OA in the remote FT is on the order of 10 days. This is significantly shorter than the FT lifetime assuming just wet and dry deposition as the primary loss mechanisms (~50 days in GEOS-Chem v10), and suggests a chemical removal mechanism, likely heterogeneous OH oxidation, possibly with a contribution from photolysis. This provides a key constraint for modeling of OA in the FT, based solely on measurements. The likelihood of different chemical removal mechanisms and their implementation and validation in a global model (GEOSChem v11) will be discussed. The contributions of methanesulfonic acid (MSA) and particulate organic nitrates ($pRONO_2$) to total OA in the remote troposphere will be discussed as well.

12AC.2

Effects of Temperature on Nucleated Particles from α-Pinene Ozonolysis Measured by a FIGAERO-Chemical Ionization Mass Spectrometer. QING YE, Mingyi Wang, Victoria Hofbauer, Dexian Chen, Jasper Kirkby, Neil Donahue, CLOUD Collaboration, *Carnegie Mellon University*

Oxidation products from α-pinene ozonolysis form particles that will scatter sunlight and nucleate clouds. These products, formed via various reaction pathways under different environmental conditions, have a wide range of volatilities and structures that will determine both their gas-particle phase partitioning and their tendency to participate in condensed phase reactions. It has been shown that highly oxygenated multifunctional molecules (HOMs) from α-pinene ozonolysis contribute to nucleation and particle initial growth. Thus understanding the formation of HOMs is crucial to constrain particle loading in the pre-industrial atmosphere. Recent research shows that HOMs are formed via autooxidation process where highly oxygenated RO_2 radicals are formed through multiple cycles of intramolecular hydrogen abstraction and O_2 addition to the initial RO_2 radicals from α-pinene ozonolysis. The autooxidation process, which is a unimolecular reaction, is strongly temperature dependent, and low temperature slows down the autooxidation rate. Therefore, nucleation and initial particle growth is expected to reduce. On the other hand, low temperature favors condensation of materials with higher volatilities (semi-volatiles become low-volatiles and low-volatiles become extremely low-volatiles at low temperature), which are presumably less polar and oxygenated. Thus, composition and properties of the nucleated particles at different temperatures could be very different.

Chemical ionization mass spectrometry coupled with a filter inlet for gas and aerosols (FIGAERO-LToF-CIMS) can measure the chemical composition of gas and condensed phase products from α-pinene ozonolysis with high time resolution and high mass resolution. We deployed a FIGAERO-LToF-CIMS with iodide as the reagent ion in the experiments in the Cosmics Leaving Outdoor Droplets (CLOUD) chamber at CERN. In the experiments, particles were formed through pure organic nucleation under 3 different temperatures, 25^{o}C, 5^{o}C and -50^{o}C with 600 ppt α-pinene and 40 ppb ozone without the addition of NO_x and under dark conditions. When gas phase products were analyzed by the CIMS, particle phase products were being collected on the Teflon filter for 30 mins. During the particle measurement mode, the filter was heated up to 170^{o}C from room temperature to evaporate materials collected on the filter and the materials were then analyzed by the mass spectrometer.

Our preliminary results show that we are able to clearly measure the monomers (C8−10 compounds) and dimers (C16−20 compounds) in the particle phase under all temperatures in our experiments. At 5^{o}C, both the monomers and dimers mass range contain products with higher oxygen number than at -50^{o}C, and the overall O/C is higher at 5^{o}C than at -50^{o}C. At 25^{o}C, oxidized products in the particles contain molecules with 6 oxygens or more while at -50^{o}C, molecules with 3 oxygens start to appear in the particles phase. In addition, we observed more fragmentation (increased fraction of C8−9 compounds in monomers and increased fraction of C16−19 compounds in dimers) at higher temperature than at low temperature. Our work will provide better understanding on particle formation and properties of the nucleated particles from α-pinene ozonolysis at different atmospheric temperature conditions.

12AC.3

The Role of Biological Particles in the Amazon Rainforest. SWARUP CHINA, Susannah Burrows, Marje Prank, Daniel Veghte, Bingbing Wang, Johannes Weis, Natalie Mahowald, Daniel Knopf, Mary Gilles, Alexander Laskin, *Pacific Northwest National Laboratory*

The Amazon basin is the largest rainforest on Earth, and therefore plays a major role in global biogeochemical cycles as well as the global water cycle. Improved understanding of the Amazon rainforest's interactions with the atmosphere is therefore a topic of interest. These interactions the particulates emitted from, and deposited to the Amazon rainforest, as players in global nutrient transport and as sources of cloud condensation and ice nuclei. Locally emitted biological particles dominate the coarse mode aerosol particle population in the basin. Particles with mixed sodium salts observed in the area are commonly attributed to marine aerosols transported from the Atlantic Ocean. Here, using detailed chemical imaging analysis and modeling studies, we show that biological particles emitted by the forest biosphere are a major source of sodium-containing particles observed in the central Amazon basin, likely the dominant source of particulate sodium during the wet season. Furthermore, we show that a significant fraction of biological particles is internally mixed with submicron- to micron-sized dust particles. Dynamic microscopic observations of ice nucleation events on individual biological-dust particles reveal that water uptake and ice formation is initiated by the dust inclusions of the mixed biological-dust particle rather than the carbonaceous material of biological particles. Our results suggest that dust inclusions may plausibly impact cold cloud formation in Amazonia and thus influence the cloud microphysics and hydrological cycle in the Amazon basin.

12AC.4

Photochemical Aging and Transformation of Dissolved Organic Matter in Atmospheric Aqueous Phase. QI ZHANG, Lu Yu, Wenqing Jiang, *University of California, Davis*

Dissolved organic matter (DOM) is a significant constituent of fog and cloud waters resulting from dissolution of water-soluble organic particles and gases. DOM can undergo aqueous reactions to form more oxidized and less volatile species, which can significantly influence ambient organic aerosol (OA) concentration and composition after water is evaporated from drops. Studying the reactions of DOM in atmospheric waters is thus important for understanding the aqueous-phase aging and processing of OA. In this study, fog waters collected in the Central Valley of California during winter are illuminated with simulated sunlight while the evolution of DOM composition is characterized using an Aerodyne High-Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-AMS) and a total carbon analyzer. Over the course of illumination equivalent to several days of tropospheric aging, the mass concentration of DOMOA (i.e., low-volatility DOM in fog water) increases, along with a gradual increase of DOMOA oxidation. The nitrogen-to-carbon ratio (N/C) of DOMOA also increases, indicating the formation of organic nitrogen compounds as well. However, the organic carbon concentration in the fog water remain constant throughout the reaction period, indicating that the increase of DOMOA is fully attributed to functionalization reactions that incorporate oxygen- and nitrogen-containing functional groups into the molecules. In the meantime, since the average molecular weight of DOMOA appears to decrease during the reactions, fragmentation reactions also happen but do not lead to significant formation of VOCs. Analysis of the HR-AMS mass spectra of DOMOA using Positive matrix factorization (PMF) allows us to represent the aqueous aging of DOMOA as a linear combination of the dynamic variations of distinct factors. The mass spectra and the time series of the factors yield insights into the aqueous phase aging process of organic matter in atmospheric condensed phases.

12AC.5

An Anthropogenic Source of Organo-nitrate from Alberta Oil Sands Emissions. ALEX LEE, Max Adam, John Liggio, Shao-Meng Li, Megan Willis, Jonathan Abbatt, Travis Tokarek, Charles Odame-Ankrah, Jennifer Huo, Hans Osthoff, Kevin Strawbridge, Jeff Brook, *National University of Singapore*

The emissions from oil sands operations have been the subject of recent studies due to the potential impacts on air quality and climate. In particular, substantial production of secondary organic aerosol (SOA) has been recently reported downwind of Alberta oil sands operations. Although intermediate volatile organic compounds (IVOCs) released from these operations have been shown to be important precursors of the observed SOA, the formation mechanisms and the chemical characteristics of such SOA remain poorly understood.

In this work, we provide evidence that emissions from Alberta oil sands operations result in the formation of large amounts of particle-phase organonitrate (ON) due to the daytime chemistry of IVOCs in the presence of NOx. High-resolution aerosol mass spectrometers (HR-AMS) were deployed in both ground-based and aircraft studies to measure the chemical compositions of non-refractory particulate matter (NR-PM, including, ammonium, nitrate, sulfate, chloride and organic) in August and September, 2013. While the ground observations identified potential sources of organic aerosol (OA) due to various industrial activities in the oil sands region, the flight tracks of aircraft measurements were designed to trace the chemical evolution of OA within the plumes downstream from the oil sands facilities.

Using the –log(NOx/NOy) as a proxy of photochemical age, positive matrix factorization (PMF) of OA fragments identified a fresh SOA factor that contributed approximately 32 wt% of the total OA at the ground site, and was associated with IVOCs measured by the co-located gas-chromatograph-ion trap mass spectrometer. This fresh SOA factor was strongly correlated to the total nitrate (i.e., nitrate salts plus organo-nitrate, r2 > 0.8). The high nitrate fragments ratio (i.e., NO+/NO2+) indicates a significant contribution of ON to the total nitrate, and our estimations suggest that ON could account for up to ~50 wt% of the fresh SOA material. Diurnal patterns of the fresh SOA, nitrate, and NOx showed local peaks at approximately 10:00 and 13:00, suggesting that the observed ON was predominantly produced via photochemistry in the presence of NOx.

The aircraft measurements also observed a strong correlation between ON and OA mass loadings within the plumes that were dominated by the fresh SOA component produced through photochemistry. Using the top-down emission rate retrieval algorithm (TERRA), our preliminary results indicate that the ON production rate in a particular plume was approximately 15 tonnes per day during the summer. In addition to the above observations, photooxiation laboratory experiments were carried out to explore the formation of ON using IVOCs from bitumen vapor as SOA precursors under high NOx conditions. High ON-to-SOA ratios (~0.3-0.5) were observed in the flow tube experiments with an estimated photochemical age of 1-3 days, which are largely consistent with our field observations. Although nocturnal chemistry of nitrate radical and biogenic VOCs has been recognized as significant sources of ON in the atmosphere, our findings highlight the significance of anthropogenic ON production via photochemistry in crude oil production and refining region worldwide.

12AC.6

A Multi-Site Chemical Characterization of Organic Aerosol Demonstrates Extensive Variability in Molecular-Level Composition. DREW GENTNER, Jenna Ditto, Emily Barnes, Peeyush Khare, Taekyu Joo, Masayuki Takeuchi, Gamze Eris, Nga Lee Ng, Alexander Bui, Robert Griffin, *Yale University*

The lifecycles of organic compounds in the atmosphere occur amongst the evolution of a remarkably diverse complex mixture of 10,000's of compounds spread across volatility and polarity scales. Yet, its molecular-level chemical composition is key to its transformations, fates, and impacts; and is essential to understanding and modeling the dynamics of complex organic aerosol mixtures in the atmosphere. Using liquid chromatography and very-high resolution mass spectrometry with "soft" ionization, we perform a detailed molecular-level characterization and intercomparison of oxidized organic aerosol from 3 very different field sites and an oxidation chamber. Despite similar aerosol bulk properties measured by multiple instruments, we report very large day-to-day molecular-level variability between ambient organic aerosol samples at each of the 3 sites, with 57-94% of compounds being unique sample-to-sample. Chamber experiments with small variations confirm this variability could be due to emitted precursor mixtures and/or chemical oxidation pathways, which is further supported by 0-D chemical modeling. In contrast to less speciated measurements, these results demonstrate much greater variability in the atmosphere under roughly similar conditions, which has implications for fundamental studies and air quality-climate models.

12AC.7

Chemistry and Photochemistry at the Surface of Tomorrow's Urban Particulate Matter. SARAH STYLER, Maya Abou-Ghanem, Stephanie Schneider, Zhihao Chen, Ming Lyu, Brett Wickware, Jonathan Abbatt, Patrick Milner, Arthur Duarte de Marins Costa, Jeffery Kwasny, *University of Alberta*

In both Canada and the United States, the largest anthropogenic source of primary $PM_{2.5}$ is dust resuspension from paved and unpaved roads. Since road dust contains many toxic species, including heavy metals and polycyclic aromatic hydrocarbons, many studies have focused on its composition and potential health effects. By contrast, little is currently known regarding its atmospheric reactivity.

We have previously shown that illumination of urban road dust leads to the production of singlet oxygen ($^1O_2$), an important environmental oxidant. Here, we report spatial and seasonal variations in $^1O_2$ production by road dust, and thereby provide new insights into the relationship between road dust composition and photochemical reactivity. We also present results from coated-wall flow tube investigations of ozone and NO_2 uptake by winter street sweepings and brake wear particles.

As vehicle exhaust emission regulations become more strict in coming years, the relative contribution of road dust and other non-exhaust emissions to urban PM loadings will increase. Our work provides evidence that photochemistry at the surface of road-derived PM can influence both the lifetimes of pollutants present at the dust surface and the composition of the surrounding atmosphere.

12AC.8

The Role of Criegee Intermediates in Secondary Sulfate Aerosols Formation in Nocturnal Power-Plant Plumes in South Eastern USA. Daphne Meidan, Steven S. Brown, YINON RUDICH, *Weizmann Institute of Science*

Criegee Intermediates from ozonolysis of biogenic volatile organic compounds (BVOC) have been suggested to be important atmospheric oxidants. However, due to low atmospheric concentrations, possible high reactivity with water vapor, SO_2, NO_2 and unconstrained thermal decomposition rates, their impact on the atmosphere remains largely unidentified.

In this study, we investigate the formation of Secondary Sulfate Aerosols (SSA) in nocturnal power plant plumes in the South-Eastern USA, which is characterized by high background of BVOCs. At these conditions (high SO_2, NO_x, BVOCs concentrations and no photochemical OH) CI reactions may contribute to the formation of SSA. Under the high concentrations of SO_2 in power plant plumes, the CI + SO_2 reaction can compete with other pathways, such as water vapor reactions and thermal decomposition. In such cases it is possible to test the current understanding of the role of CI in SO_2 oxidation that can then be extrapolated to the broader atmosphere.

We will present a dispersion model that includes nighttime and CI gas phase chemistry to simulate plume evolution during nighttime. The model results are compared to aircraft measurements of different power-plant plumes to evaluate the primary-secondary ratio and the CI impact on the SSA.

The results suggest that despite a high background of primary sulfate aerosols, Secondary Sulfate Aerosols formation increases by a factor of 3.5 when considering the CI contribution, accounting to up to 35% of the total sulfate aerosol in the plume. This effect decreases when the thermal decomposition rate is set to the higher measured CH2OO rate, 200 s^{-1} yet the CI chemistry still contributes to SSA formation through the additional OH produced in the CI thermal decomposition. These results may change if different rate coefficients for different CI's are considered. The most important CI is the C1 (CH_2OO) that consists up to 50% of the CI's produced from isoprene. C4 CI's may consist up to 45% of the CI's produced and are expected to have much slower thermal decomposition rates and water reaction rate coefficients. This suggests that the model results presented here may be a lower limit to the CI contribution to SSA.

12AP.1

Scaling Laws for Light Absorption by Atmospheric Black Carbon Aerosol. RAJAN K. CHAKRABARTY, William Heinson, *Washington University in St. Louis*

Black carbon (BC) aerosol, the strongest absorber of visible solar radiation in the atmosphere, contributes to a large uncertainty in direct radiative forcing estimates. A primary reason for this uncertainty is inaccurate parameterizations of BC mass absorption cross-section (MACBC) and its enhancement factor (EMACBC)–resulting from internal mixing with non-refractory and non-light absorbing materials such as sulfates, nitrates, and organic carbon–in climate models. Electromagnetic wave interaction with BC aerosol is a complex problem involving the non-Euclidean particle morphologies that dynamically change with variations in mixing states. Here, applying scaling theory to numerically-exact electromagnetic calculations of simulated BC particles and observational data on BC light absorption, we show that MACBC and EMACBC evolve with increasing internal mixing ratios in simple power-law exponents of -1/3. Remarkably, MACBC remains inversely proportional to wavelength at any mixing ratio. When mixing states are represented using mass-equivalent core-shell spheres, as is done in current climate models, it results in significant under prediction of MACBC. We elucidate the responsible mechanism based on shielding of photons by a sphere’s skin depth. Together, our results hold promise for accurately and inexpensively parameterizing the non-equilibrium process of BC light absorption in models and satellite retrieval algorithms.

12AP.2

Properties and Mixing State of Refractory Black Carbon over the Amazon Basin. BRUNA A. HOLANDA, Christopher Pöhlker, Henrique Barbosa, Joel Brito, Samara Carbone, Yafang Cheng, Florian Ditas, Jeannine Ditas, Thomas Klimach, Christoph Knote, Luiz Machado, Jing Ming, Daniel Moran-Zuloaga, Mira L. Pöhlker, Maria Prass, Jorge Saturno, Hang Su, David Walter, Qiaoqiao Wang, Paulo Artaxo, Ulrich Pöschl, Meinrat O. Andreae, *Max Planck Institute for Chemistry, Mainz, Germany*

Black carbon (BC) accounts for a significant fraction of the atmospheric aerosol burden and efficiently absorbs shortwave radiation with direct effects on the Earth's radiation budget[1]. Additionally, BC-containing particles can act as cloud condensation nuclei (CCN) and influence cloud microphysics (indirect effect), or even affect cloudiness when advected above the boundary layer (semi-direct effect). These effects can be amplified by internally mixing with other non-absorbing compounds. In recent times, the widespread burning of savanna vegetation and tropical forests in Africa and South America represents one of the major sources of BC to the atmosphere globally[1].

Here we present long-term measurements of BC particles at the Amazon Tall Tower Observatory (ATTO), located ~150 km northeast of Manaus, Brazil[2]. The research site is a unique platform for studying near-pristine atmospheric conditions in contrast to anthropogenic pollution. The characterization of BC particles is done using a Single Particle Soot Photometer (SP2) instrument that directly measures the mass of individual refractory BC particles (rBC), from which can be calculated their size and associated coatings. Furthermore, aircraft measurements during the ACRIDICON-CHUVA field campaign characterized rBC over large areas of the Amazon basin during the dry season of 2014[3], including direct observations of fresh biomass-burning (BB) plumes.

Aircraft measurements identified a pronounced gradient in regional rBC concentrations, typically increasing from northwestern (more pristine) to the southeastern (more influenced by regional fires) Amazon region. Moreover, most of the rBC is located in the lower 4 km of the atmosphere. In the upper troposphere (> 8 km), rBC concentrations were only a few nanograms per cubic meter, with exception of some outflow regions. In the Amazon, deep convection can be responsible for the updraft of rBC particles from the lower troposphere to higher altitudes, especially in regions heavily impacted by BB emissions. In addition to the local BB emissions, an extended pollution layer enriched in BC particles (up to 2 µg/m3, stp) was found at ~3.5 km altitude, transporting BB aerosol from Africa to the Amazon basin. Within the pollution layer, the rBC cores that have aged for at least 10 days during transatlantic transport, are larger than the ones observed in local fresh BB plumes.

In this study, we relied on vertically and spatially resolved rBC measurements to determine the microphysical properties of rBC particles over the Amazon according to the different emission sources and transport time. Moreover, using long-term observations at ATTO we try to investigate to what extent they affect aerosol cycling and, ultimately, regional climate in this complex ecosystem.

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12AP.3

Morphology and Mobility Diameter of Carbonaceous Aerosols during Agglomeration and Surface Growth. EIRINI GOUDELI, Georgios Kelesidis, Sotiris E. Pratsinis, *University of Minnesota*

Combustion is essential to the manufacture of carbon black, fumed oxides, optical fibers and high-value products, like carbon nanotubes. Carbon black is the largest flame-made nanostructured material by volume and value. Similarly to soot, a major air pollutant, carbon black particles have irregular, fractal-like structure, consisting of chemically-bonded and polydisperse primary particles. The morphology of carbon black determines its end-use and performance in nanocomposites (e.g. tires) or battery electrodes. The mobility size estimation of such evolving fractal-like aggregates is not trivial, as it depends on their structure as well as the number and size of their constituent primary particles. Scaling laws describing the mobility size of agglomerates consisting of monodisperse primary particles in point contact have been developed in the free molecular, transition and continuum regimes. However, these models overestimate up to 37% the mobility diameter of mature soot aggregates as they neglect primary particle polydispersity.

Here nascent soot dynamics, after nucleation or inception, are investigated by Discrete Element Modeling (DEM) from free molecular to transition regime. During nascent soot formation, polydisperse spheres and aggregates are formed by agglomeration and surface growth, attaining an asymptotic geometric standard deviation of 1.2 ± 0.01, in agreement with experiments in premixed, diffusion flames and wood combustion. When surface growth stops, mature soot grows by agglomeration of these polydisperse spheres and aggregates before oxidation and condensation take over. The evolution of nascent soot structure from spheres to aggregates is quantified by the mass fractal dimension and mass–mobility exponent, in excellent agreement with microscopic and mass–mobility measurements in a standard burner-stabilized stagnation ethylene flame. Based on aggregate projected area, a scaling law is derived for determining the primary particle size of nascent soot aggregates from mass–mobility measurements rather than tedious image counting. Furthermore, easy-to-use relationships between the mobility diameter and the average number of primary particles per agglomerate as well as the relative effective density of soot are proposed.

12AP.4

The Effect of Electric Field Induced Alignment on the Electrical Mobility of Fractal Aggregates. JAMES CORSON, George Mulholland, Michael Zachariah, *University of Maryland*

We study the effects of electric field strength on the mobility of soot-like fractal aggregates (fractal dimension of 1.78). The probability distribution for the particle orientation is governed by the ratio of the interaction energy between the electric field and the induced dipole in the particle to the energy associated with Brownian forces in the surrounding medium. We use our extended Kirkwood-Riseman method to calculate the friction tensor for aggregates of up to 2000 spheres, with primary sphere sizes in the transition and near free molecule regimes. Our results for electrical mobility versus field strength are in good agreement with published experimental data for soot, which show an increase in mobility on the order of 8% from random to aligned orientations. Our calculations show that particles become aligned at decreasing field strength as particle size increases because particle polarizability increases with volume. Large aggregates are at least partially aligned at field strengths below 1000 V/cm, though the small change in mobility means that alignment is not an issue in many practical applications. However, improved DMAs would be required to take advantage of small changes in mobility to provide shape characterization.

12AP.5

Light Scattering and Absorption by Fractal Aggregates Including Soot. CHRISTOPHER SORENSEN, Jerome Yon, Fengshan Liu, Justin Maughan, William Heinson, Matthew Berg, *Kansas State University*

The problem of how fractal aggregates, and in particular soot fractal aggregates, scatter and absorb light is important in many applications ranging from in situ diagnostics of soot formation in flames to the radiative effects on the global environment. The foundational description for fractal aggregate scattering and absorption is the RDG fractal aggregate (RDGFA) theory which assumes that the light interacts with the aggregate so weakly that there is no internal coupling, or equivalently, no internal multiple scattering within the aggregate [1].

Here we address the question of how well the RDGFA describes fractal aggregate scattering and absorption. This has been addressed extensively in the past but never in a comprehensive, systematic manner which we provide here. We restrict our study to DLCA fractals with a fractal dimension of 1.8. Two monomer size parameters, 0.157 and 0.314, were studied and the number of monomers per aggregate ranged from 1 to 503. The optical properties studied were the forward scattering intensity, the angular scattering as parameterized by the scattering wave vector and the total absorption cross section. We find deviations from RDGFA of ca. 10 to 40% increasing with monomer size and monomer refractive index real part, decreasing with refractive index imaginary part, and fairly constant with aggregate size.

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12AP.6

Sensitivity of Bare Black Carbon MAC and AAE to Morphological Parameters, Primary Particle Polydispersity, and Refractive Index in the Visible and Near-Infrared. FENGSHAN LIU, Jerome Yon, José Morán, Andrés Fuentes, Joel Corbin, Prem Lobo, Gregory Smallwood, *National Research Council Canada*

The mass absorption cross section (MAC) and Ångström absorption exponent (AAE) in the visible and near-infrared spectrum are important optical properties of freshly emitted black carbon (BC) (also called soot) particles. These optical properties are required in climate modeling and in the real-time BC mass concentration measurement through conversion of BC absorption coefficient measured by optically based instruments, such as the cavity-attenuated phase shift (CAPS) PM_{SSA} monitor and the photoacoustic extinctiometer (PAX). The basis of conducting BC mass concentration measurements using CAPS and PAX and other similar instruments is the assumption that MAC and AAE are fairly robust. Although the effects of certain parameters, such as the fractal dimension Df, aggregate size Np, and refractive index m, on the radiative properties of bare BC aggregates have been investigated previously, there is a lack of systematic understanding on how morphological parameters, primary particle size distribution, and refractive index affect MAC and AAE of BC aggregates.

In this study the optical properties of BC aggregates, especially the absorption cross sections required to derive MAC and AAE, are computed for numerical fractal aggregates generated using the diffusion-limited cluster aggregation (DLCA) algorithm and tunable cluster-cluster aggregation (CCA) algorithms when the effect of a specific parameter is investigated. The morphological parameters (Df, kf, dp, and Np) considered in this study are relevant to combustion-generated BC particles and different refractive indices available in the literature in the visible and near infrared spectral region (400 to 1100 nm). In addition, the potential importance of primary particle polydispersity is also investigated by generating fractal aggregates formed by lognormally distributed primary particles. The optical properties of BC fractal aggregates are calculated using the generalized Mie-solution method (GMM) and the discrete dipole approximate (DDA). The objective of this study is to quantitatively understand how the morphological parameters, primary particle size distribution, and the refractive index affect the theoretical MAC and AAE.

Since the degree of internal multiple scattering within aggregate is dependent on all the parameters considered, i.e., the morphological parameters, primary particle size distribution, refractive index, and wavelength, it is anticipated that MAC and AAE will display different degrees of departure from the Rayleigh-Debye-Gans (RDG) approximation results. The results of this study will demonstrate that the MAC and AAE of BC aggregates are not unique, but dependent on the morphological parameters, primary particle size distribution, and the refractive index. Comparison between the computed MAC and available measured MAC at specific wavelengths will also be made.

12AP.7

Fragmentation of Synthetic Fractal-like Agglomerates via Random Binary Scission. Lorenzo Isella, Anastasios D. Melas, Margaritis Kostoglou, YANNIS DROSSINOS, *European Commission, Joint Research Centre*

Particle transport depends sensitively on the particle size distribution and its time evolution via, for example, coagulation or agglomeration and fragmentation. Whereas the dynamics of particle agglomeration, driven, for example, by thermal motion, and the structure of the resulting agglomerates have been extensively studied, the fragmentation of fractal-like agglomerates has not received adequate attention.

We consider morphology-dependent linear fragmentation of synthetic fractal-like agglomerates. Loop-less, power-law agglomerates were generated by a modified tunable cluster-cluster aggregation algorithm that generates agglomerates of specified fractal prefactor and dimension, composed of arbitrary number (size) of spherical, identical, and point-touching monomers.

The simulated fragmentation process is based on mapping the initial agglomerate onto a symmetric adjacency matrix. The adjacency matrix is constructed from all the monomer-monomer Euclidean distances: monomer-monomer links (bonds) are represented by one and the absence of a link by a zero. The binary adjacency matrix, as suggested by graph theory, may be used to determine the connected components (fragments) of a structure. Given the adjacency matrix associated with an agglomerate, a link is randomly removed, according to a uniform probability distribution. The connected components of the resulting structure are determined. If the initial agglomerate fragments, the sizes of the fragments are stored. Only one link is removed per agglomerate, no multiple fragmentation events were considered.

We generated clusters of fractal prefactor 1.3 and variable fractal dimension (1.6, 1.8, 2.1). Their number and size varied from generation 4 clusters (83 to 110 monomers) to generation 7 clusters (730 to 810 monomers) for a total of approximately 400,000 clusters per fractal dimension. We numerically determined the size distribution of the fragments arising from the fragmentation of an initial N-monomer cluster. We found that the fragment size distribution peaks at the smallest (one monomer) and largest (N-1 monomers) fragments: a symmetric U-shaped fragment size distribution was observed.

The modelled fragment size distribution must obey two (inter-related) conservation laws. Mass conservation requires that the sum of monomers in the fragments must equal the number of monomers in the initial agglomerate. Moreover, the expected number of clusters arising from the binary fragmentation of an agglomerate should be two, and their distribution symmetric.

The fragmentation kernel was expressed as the product of the fragmentation rate of an initial agglomerate of size y times the fragment size distribution, i.e., the distribution of particles of size x arising from the break up of a particle of initial size y. For the time-independent fragmentation mechanism we considered, the fragmentation rate was taken to be constant, rendering the fragmentation kernel proportional to the fragment size distribution.

We modelled the homogeneous fragmentation kernel as the properly normalized product of the Brownian coagulation kernel of two fractal-like agglomerates times the beta distribution. The beta distribution models the product of fragment sizes x(y-x) raised to a (negative) power. The proposed empirical fragmentation kernel compares favourably well with the numerical fragment size distribution and with previously proposed U-shaped fragmentation kernels. The effect of the morphology of the initial agglomerate, as described by its fractal dimension, was also studied. We found that the straight-chain limit, uniform fragment size distribution, is reached only for fractal dimensions very close to unity.

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12AP.8

Spatio-Temporal Variability of Aerosol Physical and Optical Properties from Mobile In-Situ Measurements in the Po Valley (Italy) during Summertime. MICHELE BERTÓ, Rosaria Erika Pileci, Robin Modini, Stefania Gilardoni, Angela Marinoni, Douglas Orsini, Matteo Rinaldi, Martin Gysel, *Paul Scherrer Institute*

Characterizing the spatio-temporal variability of atmospheric aerosols in terms of physical and optical properties is of great importance in evaluating their climatic and health effects. Black carbon (BC) particles have mainly anthropogenic origin and they are the main light absorbing component of the atmospheric aerosol. BC has the second largest positive radiative forcing value (RF), but with an uncertainty of 90%. A still poor knowledge of the mass absorption cross-section (MAC, the ratio between the absorption coefficient and the mass concentration of BC) spatio-temporal variability, absolute value and its behaviour in terms of coating absorption enhancement, significantly contribute to BC RF uncertainties.

To investigate the BC MAC variability and its relations with other aerosol physical and optical properties, a field campaign ("Actris-2 - Mt. Cimone and Po valley field campaign 2017") was carried out in July by using a mobile pollutants measurement laboratory equipped with several scientific instruments, among others a Single Particle Soot Photometer (SP2, DMT) and a Multiangle Absorption Photometer (MAAP, Thermofisher). Four environmental pollutants regimes were characterized: urban traffic (streets), urban background (CNR, Bologna), rural areas and a high altitude location (Mt. Cimone).

A MAC diurnal cycle was observed during stationary measurement at CNR: MAC minimum occurring in the morning when fresh traffic emissions dominated, maximal values in the afternoon when BC mass was dominated by aged particles. The coating-induced lensing effect is the hypothetical explanation for the MAC increase. Traffic emissions were an important factor in explaining the variability in MAC values during the mobile measurements causing a decrease in the MAC absolute values, otherwise generally stable due to the mostly aged particles in the Po Valley troposphere. Further quantitative investigation of BC core/coating diameters is planned to provide a clearer explanation of the MAC variability.

12BA.1

Indoor and Outdoor Concentrations of Airborne Microbes (Bacteria and Fungal Spores) in a Hot Desert Environment.

BALINT ALFOLDY, Lubna Ali, Mariem Safi, Mohamed Kotb, Nahla Eltai, Jeffrey Obbard, *Qatar University*

The airborne transmissions of pathogens, non-pathogenic organisms, fragments of microbial cells, and byproducts of microbial metabolism, collectively referred as “bioaerosols” represent a potential risk to human health upon inhalation in both outdoor and indoor environments. Outdoors, microbes may be derived from a variety of sources including soils, vegetation and animals, whilst indoors sources include infected individuals who emit pathogenic microbes via coughing, sneezing and perspiration. Normal activities of healthy individuals can also contribute to the airborne microbe level via exhalation and skin cell degeneration. Furniture, carpets, food debris and pets are also important sources of microbes. The indoor levels of airborne microbes is a function of occupant density, duration of room occupation, presence of any infected individuals, and the degree of ventilation and air-exchange with the outdoor environment. The ventilation system itself may also serve as a source of airborne microbes in the case if it is not properly maintained.

The aim of this study was to investigate the quantity, size distribution and species of airborne microbes inside a school classroom, as well as in a hot, desert outdoor environment, in Doha, Qatar. Air samples were collected simultaneously indoors and outdoors during several sampling periods i.e. summer, autumn, winter and spring. An Anderson six-stage impactor was used to collect airborne microbes on nutrient agar (NA) plates by 30 l/min flowrate, over a 5 minutes period, i.e. total 150 liters of air collected per sample. Air samples were collected in triplicate both indoors and outdoors prior to commencement of class at 6:30 AM, and immediately after end of classes at 2:30 PM. After sampling, NA plates were then incubated for 24 hours at 37°C. After incubation the number of colony forming units (CFU) of microbes on the NA plates were counted, and the average of triplicate samples for the morning and afternoon samples were calculated as the mean number of airborne microbes per cubic meter of air (CFU/m^3).

The prevalence and concentration of microbes varied spatially (indoors versus outdoors), temporally (morning versus afternoon), and seasonally (winter versus summer). The concentrations of airborne bacteria in classroom air were lowest in the morning (a maximum 204 CFU/m^3 in summer, and a maximum 35 CFU/m^3 in winter) than in the afternoon after class (a maximum 348 CFU/m^3 in summer, and a maximum 543 CFU/m^3 in winter). As the classroom was continuously occupied between the morning and afternoon, then human influence is the most likely factor affecting prevailing CFU levels. Other factors likely affecting CFU levels may include: airflow dynamics and exchange between the indoor and outdoor environment; the influence of the classroom air-conditioning and ventilation system (positive or negative) and; the presence of non-human bacterial sources in the classroom (food debris, carpeting, soft furnishings etc.).

Outdoor air samples showed the opposite profile to the classroom, where morning samples had higher numbers of airborne microbes in the morning (a maximum 640 CFU/m^3 in summer, and a maximum 111 CFU/m^3 in winter) compared to the afternoon samples (a maximum 299 CFU/m^3 in summer, and a maximum 82 CFU/m^3 in winter). This contrast supports the indication that airborne bacteria in the classroom are derived from internal sources rather than as a result of infiltration of bacteria from outside.

12BA.2

Variation of Microbial Community and Activity in PM2.5 in Beijing, China. RUI DU, Weishan Ren, Pengrui Du, Hanlin Chen, Sujian Zhang, *University of Chinese Academy of Sciences*

Bacteria and fungi are primary constituents of airborne microbes in fine particulate matter ($PM_{2.5}$) and significantly impact human health. However, hitherto, seasonal variation and effect of air pollution on microbial community composition and microbial activity are poorly understood. This study analyzed the bacterial and fungal composition of $PM_{2.5}$ using gene sequencing methods. Furthermore, The fluorescein diacetate (FDA) hydrolysis method was also tested the microbial activity in atmospheric $PM_{2.5}$ under different air pollution levels during different seasons in suburban Beijing. The results showed that the species richness and diversity of bacterial communities displayed a downtrend with the aggravation of air pollution. Additionally, the bacterial communities in spring samples showed the highest species richness, with average richness estimators, ACE and Chao 1, up to 14649 and 7608, respectively, followed by winter samples (7690 and 5031, respectively) and autumn samples (4368 and 3438, respectively), whereas summer samples exhibited the lowest average ACE and Chao 1 indexes (2916 and 1900, respectively). The species richness of fungal communities followed the same seasonal pattern. Pathogenic fungi were more abundant in winter than other seasons, but, there were no significant differences about the pathogenic bacteria and fungi under different air quality levels. In addition, the microbial activity in atmospheric $PM_{2.5}$ under excellent and good air quality level was usually at the peak in different seasonal. Yet, the highest value was exhibited under good air quality level instead of under excellent level. Moreover, the microbial activity showed a downtrend with the aggravation of air pollution except for the strong heavy pollution level(AQI between 300-500). Surprisingly, the winter $PM_{2.5}$ samples exhibited the top value of the microbial activity under the same air pollution level. To best of our knowledge, this is the first study that demonstrates seasonal variation characteristics of bacteria and fungi in $PM_{2.5}$ in heavy haze contaminated areas and highlights the effects of air pollution on the atmospheric microbial community. This study would be useful to other bioaerosol studies focusing on the role of the atmospheric particulate matter on human health.

Keywords: PM2.5, Microbial community and activity, Variation, Air pollution level.

12BA.3

Presence and Variability of Bioaerosols in Three Multi-Apartment Residential Buildings with Different Energy Efficiency in the Northeastern US. NIRMALA THOMAS, Leonardo Calderón, Brian Pavilonis, Zuocheng Wang, Youyou Xiong, MaryAnn Sorensen-Allacci, Deborah Plotnik, Jennifer Senick, Jie Gong, Uta Krogmann, Clinton J. Andrews, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

Presence and temporal variability of bioaerosols were studied in three multi-apartment residential buildings and correlated with building energy efficiency, socioeconomic factors, locality and environmental parameters. This analysis was part of a multiphase interventional and longitudinal study conducted to relate investigated indoor air quality parameters to residents' perception of their health and building conditions. Measurements were performed intermittently between 2011 to 2016. Building 1 is a LEED EB Platinum certified residence located in a waterfront neighborhood where 18 apartments were measured during all four seasons. Building 2 is an Energy Star certified residence with an urban rooftop garden where 15 apartments were measured during all four seasons. Building 3 is a retrofitted residence where 15 apartments were measured during the summer and 4 apartments during the winter. Each sampling day consisted of measuring bioaerosols in 1-4 apartments and taking outdoor samples.

Culturable bacteria and fungi concentrations were measured using a portable SAS Super 180 air sampler (Bioscience International, Rockville, MD) operated at 180 L/min. Trypticase soy agar (Difco, Becton, Dickinson and Co., Sparks, MD) with fungicide and malt extract agar (Difco, Becton, Dickinson and Co., Sparks, MD) were used as sampling media for bacteria and fungi, respectively. The concentration of total fungi (viable and non-viable) was determined by taking air samples with an Air-O-Cell (Zefon International, Inc., Ocala, FL) spore trap operated at 15 L/min. After sampling, the spore traps were sent to EMSL Inc. (Westmont, NJ), a certified laboratory, for speciation and quantification of the collected fungal spores.

In Building 1, concentrations of culturable fungi and bacteria in apartments ranged from 2 to 1587 #/m^3 with a median of 27 #/m^3 and from 41 to 1891 #/m^3 with a median of 230 #/m^3, respectively; winter values were lower than in summer or fall ($p<0.05$) for both variables. Outdoors fungi concentrations were higher during summer when compared to winter or spring ($p<0.005$), while outdoor bacteria samples indicated no temporal difference ($p>0.05$).

For Building 2, concentrations of culturable fungi and bacteria in apartments ranged from 2 to 718 #/m^3 with a median of 72 #/m^3 and from 24 to 4881 #/m^3 (saturation level) with a median of 226 #/m^3, respectively; winter concentrations of culturable fungi were lower than that in spring or summer ($p<0.001$). Outdoor concentrations did not vary with the season for both microorganism types ($p>0.05$).

For Building 3, concentrations of culturable fungi and bacteria in apartments ranged from 54 to 518 #/m^3 with a median of 121 #/m^3 and from 70 to 4881 #/m^3 (saturation level) with a median of 199 #/m^3, respectively; only indoor culturable bacteria concentrations were higher during summer than in winter ($p<0.05$). Outdoor fungi concentrations were higher during summer than in winter ($p<0.05$), but outdoor bacterial samples indicated no differences ($p>0.05$).

Comparison of bioaerosols concentrations among the three buildings indicated that Building 1 had the lowest concentrations of both bacteria and fungi during all four seasons except for culturable bacteria concentrations during summer. Locality and socioeconomic status played a dominant role in bioaerosol concentrations indoors. Indoor/outdoor ratios were determined, and their relationship to self-reported health concerns has been investigated. Common and distinctive fungal species at all locations were also identified. Overall, this subset of the multiphase study evaluated indoor biological air quality and related it to seasons, apartment occupancy changes, building energy efficiencies, and residents' health.

12BA.4

Online Bioaerosol and Dust Measurements during the Aqaba Research Cruise around the Arabian Peninsula. TOBIAS KÖNEMANN, Nicole Savage, Charlotte Beall, Emilio Rodriguez-Caballero, Florian Ditas, Marcel Dorf, Hartwig Harder, Jos Lelieveld, David Walter, Bettina Weber, Petya Yordanova, Meinrat O. Andreae, J. Alex Huffman, Ulrich Pöschl, Christopher Pöhlker, *Max Planck Institute for Chemistry*

The Middle East represents a hot and arid region, characterized by diverse environmental conditions ranging from near-pristine and unpolluted but dusty, to strongly polluted due to areas with high population density. A study across the region, therefore, provides a broad range of atmospheric compositions derived from both natural and anthropogenic sources. Only few comprehensive sets of atmospheric measurements have ever been performed in this region, however.

The AQABA (Air Quality and Climate Change in the Arabian BAsin) campaign, which represents one of the most comprehensive ship-borne measurement campaigns, took place from June 18th to September 3rd 2017. The majority of sampling took place from the deck of the KOMMANDOR IONA research ship, which sailed from France, across the Mediterranean Sea and the Red Sea, to Kuwait, and then back around the Arabian Peninsula to a final dock of La Seyne-sur-Mer (southern France). During the campaign, an extensive set of different measurement techniques has been applied to investigate aerosol interactions and photochemical processes. To address biological and non-biological aerosol load and composition, we performed measurements with different analytical detection techniques (e.g. Ultrafine CPC (Condensation Particle Counter) for aerosol number concentration; Wideband Integrated Bioaerosol Sensor (WIBS-4A) for fluorescent bioaerosol properties).

In addition to the instruments mentioned above, we used a novel online laser/light-induced-fluorescence instrument for real-time analysis of individual bioparticles, providing information on particle size, asymmetry, and resolved fluorescence information. The Spectral Intensity Bioaerosol Sensor (SIBS, Droplet Measurement Technologies, Longmont, CO, USA) uses two excitation wavelengths at 285 and 370 nm and resolves fluorescence emission into 16 bins, ranging from 302 to 721 nm. Particles are measured over a broad size range between ~ 0.5 and > 50 µm.

We will report first results from this pioneering field campaign and focus on the composition and properties of both biological and non-biological coarse particles over a wide variety of environmental conditions in the Middle East Region. Measurement periods included scenarios such as clean marine air, petrochemical pollution, megacity-influenced air masses, and dust from North Africa. Preliminary data indicate that the SIBS was capable of detecting scenario-specific spectral “fingerprints”, providing a certain level of particle discrimination for upcoming cluster analyses. We will show how aerosol auto-fluorescence properties can be used for online classification of bioaerosol particles.

12BA.5

A Newly Developed, Inexpensive Single-Particle Fluorescence Spectrometer: Characterization and Application to Pollen Analysis. BENJAMIN E. SWANSON, Sam Scherer, Samir Rezgui, Donald R. Huffman, J. Alex Huffman,
University of Denver, CO

Primary biological aerosol particles (PBAP) are ubiquitous throughout the Earth's atmosphere and play diverse roles in environmental systems, biological process, climate, and even human health. Bioaerosol detection in the atmosphere has historically been a time-consuming, manual process. Within the last several decades, many laser-/light-induced fluorescence (LIF) instruments have become commercially available for bioaerosol analysis. Even so, the majority of widespread identification techniques still rely on complicated analysis, as commercial instruments frequently have trouble classifying beyond broad classes of bioaerosol types (e.g. fungal spores versus pollen), and those that can perform this task are usually very expensive. Pollen-counting, for example, is frequently still accomplished via manual visual microscopy due to the costly nature or low spectral quality of UV-LIF technologies.

Here we discuss a technique we recently introduced to analyze many individual particles collected onto a glass substrate utilizing multiple excitation sources [1]. Our previous characterization work assessed the ability of the instrument to probe relevant biofluorophores within standard particles and several species of pollen used as examples [2]. Four excitation sources (280 nm, 350 nm, 405 nm, and 450 nm) were matched with emission maxima previously shown to be important for a large variety of pollen species [3]. The instrument described here can provide a quick, binary assessment of whether particles are either fluorescent or non-fluorescent, similar to the way certain commercial single-particle UV-LIF instruments are operated. Additionally, the instrument can provide resolved fluorescence spectra of individual particles at ca. 2 nm resolution. As a part of the characterization work to be shown, a method was developed to correct for defects in the inexpensive optical components and for differences in laser and LED source emission profiles. These calibration methods enable the collection of fluorescence spectra approximately normalized by particle size to help show differences in particle composition in an effort to differentiate between particle types. Despite its limit to detection of emission of wavelengths longer than 400 nm (due to limitations in the CCD detector) the instrument can confidently distinguish between species of pollen particles when employing a clustering algorithm [2]. Both K-means and Hierarchical Clustering Analysis (HAC) have been probed as possible methods of distinguishing between particles. Work has also been undertaken for automatic particle identification via a machine learning algorithm, which has shown promising results toward considerably higher particle analysis throughput.

A number of pollen species (>10) were analyzed using the clustering method, inputting full detected emission spectra (400-700 nm) and particle size measured by the instrument into a clustering algorithm. The eventual goal is to further develop a prototype handheld version of the instrument to be deployed wherever pollen or mold-spore counting and differentiation is required. This technique has demonstrated proof-of-concept ability to supplement the current host of bioaerosol LIF instrumentation at a much lower purchase-cost, while also retaining high fluorescence spectral resolution and the long-range potential to serve as a pollen-counting instrument.

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12BA.6

Computational Airflow Modeling Based Pathogen Tracking at Food Processing Facilities. Alexander Zuniga, Alejandro Castillo, Zahra Mohammad, Juan Pedro Maestre, Kerry Kinney, Ronald Lacey, MARIA KING, *Texas A&M University*

Two large beef harvesting establishments have been sampled for the presence of potentially pathogenic aerosolized bacteria during the spring and summer seasons. At each establishment, two wetted wall cyclone (WWC) bioaerosol collector units were left to continuously sample air for one day at the intensive work stations including the dehiding area and in the fabrication room with an air flow rate of 100 liters per minute. In addition, two dynamic samplers were moved along the processing line, collecting air for 4 hour periods at the various process steps, and also in the chiller room. The collected samples were tested by microbial plating for colony forming units and whole-cell qPCR method for total bacterial counts. Shiga toxin producing E. coli and Salmonella were identified using selective media and specific real-time PCR oligonucleotides. From all positive samples, DNA was extracted for microbiome analysis.

The air flow pattern of the HVAC system at the large facilities was modeled using computational fluid dynamics modeling to visualize the extent of the effect on the spread of bioaerosols, and identify any correlation between HVAC patterns and collected concentrations of bioaerosols. The facilities were modeled according to their floor plans. Experimental collection sites were correlated with the airflow by simulating the intakes of the WWC collectors at each experimental site. Other metrics such as velocity profiles and local mean age of air (LMA) were also analyzed.

Based on qPCR analysis, both plants tested positive for both Salmonella and STEC during spring and summer. The results indicated that the presence of STEC and Salmonella in the air of the meat establishments was not only dependent on the location of the physical areas where carcasses are processed, but also was dependent on the size of the plant, and the season. Significant correlation was found between the presence of STEC and Salmonella, and the size of plant, season and the area of sampling. During summer sampling, one meat establishments tested positive for Salmonella by direct plating, indicating that the bioaerosols contained relatively large numbers of pathogens. Consequently, this could lead to potential carcass contamination with fecal pathogens.

New HVAC models were created around the layout of the large facilities to create an optimized airflow pattern that will inhibit the spread of bioaerosols. For the HVAC inlet/exhaust locations at the chiller entrance from the dehiding and fabrication rooms different configurations were tested that resulted in different HVAC air flow patterns. The air flow patterns for each configuration were modeled and validated using the bioaerosol collection results to visualize the entrainment of the airborne particles. For both facilities, displacement ventilation was found to be most effective at reducing aerosol particle concentration and optimizing plant sanitation.

12BA.7

Historic and Unpublished Data on Biological Ice Nuclei: Terrestrial and Marine. RUSSELL SCHNELL, *National Oceanic and Atmospheric Adminstration*

History: By way of background, most precipitation over land (even in hot deserts) and in convective clouds over oceans, is initiated by ice crystals forming in supercooled cloud water (cloud water may supercool to -250C or colder). These freezing events are initiated by ice nuclei (IN), the best of which are of biological origin. In the late 1960s it was observed that some species of bacteria living on decaying plant litters nucleated ice at -1.30C in supercooled water drops. In the residue of well decayed plant litters a stable IN is produced that may initiate ice at -5.50C in concentrations of up to 109 at -100C per gram of litter. A sample of such decayed leaf litter collected in 1971 and stored at room temperature maintained appreciable ice nucleus activity over a 35 year period. In the marine environment, IN in plankton may nucleate supercooled water at -4.5 0C in concentrations of 108 active at -100C per gram of plankton. Some bacteria isolated from plankton are excellent sources of IN active at temperatures as warm as -30C. Natural mineral dusts free of organic particles initiate ice at much colder temperatures (-120C to -200C). As such, there is interest in determining the role of biological IN in precipitation formation.

Unpublished or Obscure Biogenic Ice Nucleus Data: In recent years a number of publications on biogenic IN show results similar to those observed up to half a century ago but unpublished or in conference proceedings and theses. Some of these earlier data may be of interest to current IN researchers. For instance, it has been observed that ocean derived IN (ODN) are better deposition IN (nucleated from supercooled water vapor) than leaf derived IN (LDN) or bacteria derived IN (BDN). But, immersion freezing activity (nucleants in water) of these biogenic nucleants show that up to 104 more IN are activated by immersion freezing than deposition freezing. In the contact freezing nucleation mode (nucleants introduced onto supercooled water), ODN exhibited more IN events than in the immersion freezing mode whereas LDN and BDN exhibited similar nucleation activity spectra in both modes. Well aged and dried LDN ground in a fluid energy mill was far superior as a contact IN than unground LDN. But, the milled LDN began to lose its advantage within hours of milling. As for IN stability, ODN can lose a majority of its IN activity within hours after being dried at room temperature. As noted above, LDN may maintain IN activity for many decades. BDN IN activity is rapidly deactivated under anaerobic stress but recovers within a few hours under an aerobic environment. Atmospheric IN measured with a combined filter and drop freezing technique has shown that atmospheric IN concentrations in Colorado are greatest in late summer and are depleted behind cold front systems that produced snow upwind of the a sampling site. Measurements of atmospheric IN in vertical profiles show higher concentrations near the surface in both terrestrial and marine environments. There are especially strong decreases above temperature inversions and above marine boundary layers compared to beneath. There are clear differences in the number and warm range IN in plant litters from different climate zones: Köppen D zones have the warmest IN and greatest concentrations per unit mass followed by C and then A zones. This is also reflected in the immersion freezing IN measured in precipitation falling in these zones. In the Sahel region of Africa during the drought of the early 1970s, IN were depleted in overgrazed regions compared to lesser grazed areas. This raises the question of what role, if any, the removal of local IN may have had in precipitation reduction?

12BA.8

Bioaerosol Investigation: New Experimental Activity in Chambre, an Atmospheric Simulation Chamber. SILVIA G. DANELLI, Dario Massabò, Elena Gatta, Franco Parodi, Antonio Comite, Gianluca Corno, Camilla Costa, Andrea Di Cesare, Maddalena Oliva, Luigi Vezzulli, Paolo Prati, *University of Genoa and INFN Genoa, Italy*

ChAMBRe (**Ch**amber for **A**erosol **M**odelling and **B**io-aerosol **Re**search, www.labfisa.ge.infn.it) is an atmospheric simulation chamber installed in Genoa (IT) and managed by the National Institute of Nuclear Physics and the Physics Department of the University. ChAMBRe is one of the nodes of the EUROCHAMP2020 network of atmospheric simulation chambers. So far, atmospheric simulation chamber have been widely used to study chemical and photochemical processes that occur in the atmosphere. However, following the tracks of a pilot experiment [1], ChAMBRe is the first chamber designed specifically for bio-aerosol studies. The chamber is made in stainless steel with a vertical cylindrical volume of about 2.2 m^3 which can be evacuated down to a residual pressure of about 2 10^{-2} mbar in about 10 minutes. The chamber is equipped with on-line monitors of the internal temperature, pressure and relative humidity. The latter can be controlled by a dedicated humidifier. The air inlet is through an absolute HEPA filter and other gas traps. UV lamps are installed both for ozone production and for sterilization purposes; a variable speed fan is placed in the bottom to favor the mixing of the internal atmosphere. Aerosol concentration and size distribution are monitored in the 5 nm - 18 µm range by both a Scanning Mobility Particle Spectrometer and an Optical Particle Counter. Wall reactivity and aerosol life time have been measured by dedicated experiments [2].

At ChAMBRe, the research on bio-aerosol is presently aiming to assess the environmental stress condition and alterations of bacteria viability when they are dispersed in the atmosphere. Basically, the microorganisms behavior is firstly studied in a clean atmosphere and later at the presence of different levels and mixing of anthropogenic pollutants, like NO_x, CO, CO_2 and Particulate Matter. According to their dimension, bacteria lifetime in ChAMBRe is sufficiently long (typically, 2 -8 hours) to allow this kind of studies. The experimental protocol consists in several consecutive steps: *in vitro* bacteria growth, injection into ChAMBRe by a Blaustein Atomizer, collection and/or sampling, laboratory analyses. By an automated shelf, several Petri dishes can be placed inside ChAMBRe for singly variable times to collect on a culture medium the suspended bacteria.

So far, the ratio between collected and injected CFU turned out to be well reproducible in a set of preliminary but systematics tests and the whole procedure to grow, inject and extract bacteria in ChAMBRE has been put on a firm ground.

During the experiment, samples can be also collected by impingers, impactors and filters. Counting of colony forming units (CFU), flow cytometry and scanning electron microscopy, are some of the off-line analyses routinely performed. Up to now, experiments were carried out on *Bacillus subtilis* and *Escherichia coli*, belonging respectively to the group of Gram-positive and Gram-negative, with the purpose to extend the analysis to other microorganisms. Results on both the bacterial strains together with a full description of the facility will be presented.

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12CB.1

High-Temperature Sampling and Characterization of Corrosion-Relevant Particles in Waste Incineration Plants.

STEFAN SCHUMACHER, Jörg Lindermann, Burkhard Stahlmecke, Dirk Jarzyna, Amit Khot, Till van der Zwaag, Hermann Nordsieck, Jens Harpeng, Ragnar Warnecke, Christof Asbach, *Institut für Energie- und Umwelttechnik e.V. (IUTA)*

Although the particulate phase in boilers of waste incineration plants has already for a long time been under suspicion to essentially drive the corrosion of the superheater tubes, it has not been comprehensively characterized to the present. This is mainly attributed to the extreme conditions present in the boilers such as high temperatures, the presence of condensable salt vapors, and high dust loads. These cause tremendous artifacts when using conventional aerosol sampling and measurement techniques that extract the aerosol from the boiler (Deuerling 2010).

Therefore, we developed a novel two stage sampling probe, which allows the collection of particles in the interesting size range from a few 10 nm up to several 100 µm and minimizes condensation artifacts (Schumacher 2016). Larger particles are sampled on an impaction plate, whereas the remaining smaller particles are collected on a nickel membrane filter with well-defined pores. Together, the broad particle size range is covered. The (aerodynamic) cut-off diameter of the impactor is between 16 and 37 µm and depends on the temperature and thus the location within the boiler, where the probe is used. The substrates are well-suited for scanning electron microscopy (SEM), which provides a comprehensive investigation of the size distribution, morphology, and chemical properties of individual particles. Using computational fluid dynamics (CFD), the collection efficiencies of the impactor as well as of the membrane filter have been studied in detail, which allows to deduce the airborne particle number and mass size distributions from counting the collected particles in SEM images. Furthermore, the probe can easily be adapted for total dust sampling and analysis (Schumacher 2017).

The probe has been successfully employed for measurements in the combustion chamber (1250°C) and the four passes (950°C down to 250°C) of two waste incineration plants with strongly different corrosion rates to characterize the evolution of the aerosol on its voyage through the boilers. On the course, the concentration of submicron particles grows by condensation of salt vapors during cooling, whereas the concentration of larger particles decreases due to deposition losses. This behavior was also modeled by CFD simulations of the particle dynamics in the boiler. We show that especially the coarse particles which have been difficult to measure up to now contain a substantial share of chlorine. Since they are efficiently deposited on the superheater tubes, deviations in this size regime might explain the different corrosion rates of the plants.

This work has been supported by the Federal Ministry of Education and Research (BMBF) within the project VOKos (Grant No 03X3589).

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12CB.2

Ultrafine Particle Emissions from the Combustion of Natural Gas, Biogas, and Biomethane. Jian Xue, Yin Li, Joshua Peppers, Peter Green, Thomas Young, MICHAEL KLEEMAN, *University of California, Davis*

Biogas and biomethane (=upgraded biogas) are major renewable fuels in the evolving energy economy. Biogas and biomethane burn cleanly but they do produce ultrafine particles (UFPs) which have greater toxicity than fine particles. The factors that control UFP emissions rates from biogas/biomethane combustion should be understood before these fuels are widely adopted.

Here we measure UFPs emissions from the combustion of biomethane and/or biogas produced from five different representative sources: two food waste digesters, two dairy waste digesters, and one landfill. Combustion exhaust for each of these biomethane/biogas sources is measured from representative sectors including electricity generation, motor vehicles, water heaters, and cooking stoves. Results show that basecase emissions of UFPs are a strong function of the sulfur content in the fuel. Sulfur content greater than 2 ppm caused a strong increase in UFP emissions. Increasing dilution during source tests caused UFPs emitted from water heaters and cooking stoves to evaporate, suggesting that these particles are semi-volatile. This may reflect the lack of ammonia in the dilution air used during the tests leading to the semi-volatile behavior of the UFPs composed mostly of sulfuric acid. UFPs from electricity generation and motor vehicles were non-volatile possibly because these particles were exposed to sufficient ammonia to produce ammonium sulfate. Photochemical aging of biomethane combustion exhaust in a representative urban “surrogate” atmosphere did not significantly alter secondary UFP formation compared to natural gas tests.

The results of the current study highlight the importance of fuel sulfur content and ammonia concentration in the background air as controlling variables for the UFP emissions rate from the combustion of natural gas, biogas, and biomethane. Future biomethane production facilities should ensure that fuel sulfur content remains below 2 ppm so that widespread adoption of biogas/biomethane does not significantly increase ambient concentrations of UFPs relative to natural gas combustion.

12CB.3

Time-resolved Monitoring of Primary Intermediate/Semi-volatile Organic Species during Coal Combustion in a Representative Household Stove in Northern China. SIYI CAI, Liang Zhu, Shuxiao Wang, Armin Wisthaler, Jiming Hao, *Tsinghua University*

Winter household coal combustion is being increasingly held responsible for air pollution in northern China. There exist knowledge gaps with respect to quantitative contribution of household coal stove emissions to SOA, and quantitative measurements of 'unconventional' I/SVOCs from coal-fired stoves are thus prerequisites. Herein, high mass resolution PTR-ToF-MS was employed to examine emission of gaseous I/SVOCs and representative VOCs from a common coal-fired stove. Five common coal samples (including three bituminous coals and two anthracite coals) were investigated. Semi-quantitative source profile of 89 primary gaseous species were presented, most of these species are identified as aromatics and oxygenated aromatics. The time-resolved evolvement of representative VOCs and I/SVOCs during one single combustion cycle as well as consecutive coal stoking process were examined. In one single combustion cycle, I/SVOCs emission during the first two stages (ignition and flaming) accounted for about 70% of the total. The average I/SVOCs emission factors of single cycle combustion is ~15% higher than that of consecutive stoking process. Dramatic differences lay between source profiles of anthracites and bituminous coals. For bituminous coal, the compounds of m/z >165 (with C# > 12) account for nearly 20% of the total organic compounds (NMOCs) observed. The same group account for only ~2% of NMOCs from anthracites.

The results of this study make an important supplement to the source spectra of I/SVOCs from household coal combustion. In other studies focusing biomass burning, the compounds in the range m/z >165 accounted for only ~1.5% of the total NMOCs emissions. Our findings indicate that residential coal combustion represent an important I/SVOC emission source than biomass burning in China. Based on available values of SOA yield, I/SVOCs is estimated to account for 40-45% of SOA formed, in the case of bituminous coals. The total NMOCs and I/SVOCs emissions from residential coal combustion are projected to 153 kt and 54 kt in north China in winter, respectively. A full transition from bituminous coal to anthracite will permit a reduction of NMOCs and I/SVOCs emissions by 97% and 99%, respectively.

Current study serves as a proof of principle case quantifying gaseous I/SVOCs from stove emissions using PTR-ToF-MS. Systematical measurements of more types of coals, various types of household stoves, partitioning of I/SVOCs between gaseous and POA phase, is to be carried out.

12CB.4

Emission Factors of PM2.5 and Its Climate Relevant Constituents from Cooking Processes in Traditional Mud Stoves in the Villages of North India. Annada Padhi, Gazala Habib, JAI PRAKASH, *IIT Delhi*

The incomplete combustion of various solid biomass fuels is central to the production of 25% of the emissions of PM2.5 and carbonaceous aerosols and about 50% of the anthropogenic emissions of carbonaceous aerosols globally. Additionally, recent studies have also shown that climate forcing emissions from residential cookstoves are not well characterized and have also strongly supported the fact that emissions data from normal daily cooking are especially sparse with most of the data derived from laboratory tests may not be representative of real-world emissions. This study presents the emission measurements carried out in the villages of western Uttar-Pradesh region of North India, where solid biomass fuel burning is pervasive throughout the year. The emission measurement was conducted during regular meal preparation in the household. It is important to note that in the villages of North India the mixture of solid biomass fuels including fuel-wood, dung-cake and crop residues is used in tradition mud stoves. Fine aerosol samples were collected on quartz filters and teflon filters with the help of a multi-stream sampler equipped with cyclone separator designed for cutoff diameter 2.5 µm at 10 lpm flow rate. The quartz filters were subjected to determine EC (elemental carbon), OC (organic carbon) and WSOC (water-soluble organic carbon) whereas teflon filters were used for determining the water-soluble ions using Ion Chromatography (Dionex 1000) following standard protocols. Mass emission factors are estimated for PM2.5 aerosols and rest of the constituents as mentioned above using the carbon balance method. The emission factors showed a strong dependence on cooking process reported process-wise such as baking, boiling, frying etc.; which in turn can be considered as a significant input to the emission estimates evaluation of these key climate pollutants as used in previous studies. A factor of 1.5 higher PM2.5 emission factors was observed from baking (3.5-1.7) gkg-1 compared to boiling (2.9-0.5) gkg-1. The emission factors measured in present work are higher than those reported from water boiling tests in the laboratory.

12CB.5

Emission Factors and Optical Properties of Health and Climate Relevant Pollutants Measured in a Multi-year Cookstove Intervention Study in Rural India. MOHAMMAD MAKSIMUL ISLAM, Roshan Wathore, Grishma Jain, Karthik Sethuraman, Hisham Zerriffi, Julian Marshall, Rob Bailis, Andrew Grieshop, *North Carolina State University*

Particulate and gaseous pollutants emitted from biomass stoves have adverse health and climatic impacts. Globally over 3 billion people, and majority of people in rural India, use solid fuel cookstoves to meet their household energy demand. Although there are studies showing alarming pollutant emissions associated with biomass stoves in the lab and field settings, there is still little real world in-home cookstove emission measurement data. Moreover, very few studies address seasonality and inter-location variability in emissions. In this study, we characterize cookstove emissions measured during a multi-year intervention study in two rural areas (Kullu in Himachal Pradesh State; Koppal in Karnataka State) in India. This study aims to find an association between adoption of alternative biomass and modern-fuel cookstoves and reduced emissions and exposures.

In the intervention, households chose from a range of stove models (e.g. advanced biomass, liquefied petroleum gas: LPG) for cooking and/or heating in homes. These stoves were typically used along with existing ones, and in-home measurements were conducted before and after selection. The study had three ~3-month-long measurement periods (baseline: BL, follow-up-1: F1, follow-up-2: F2) for each location. The time gap between measurement periods was ~7 months for each location. Most households chose to receive a modern-fuel stove (LPG, electric); fewer households (12.5% in Koppal and 32% in Kullu) selected a biomass stove. However, we conducted 129 emission measurements (54 BL; 31 F1; 44 F2) from traditional stoves (mud stoves & three-stone-fires), 55 (25 BL; 12 F1; 18 F2) from 'Tandoor' chimney stoves (Himansu Tandoor & Traditional Tandoor), 44 (4 BL; 17 F1; 23 F2) from LPG stoves, 7 from Envirofit rocket stoves and 12 from others (Prakti & TERI), totaling to 247 tests.

Emission measurements were carried out with a portable instrument (STEMS) that measures real-time concentrations of carbon dioxide, carbon monoxide (CO), particle light scattering and absorption and collects integrated filter samples for gravimetric PM2.5 and Organic/Elemental Carbon (OC/EC) analyses. Mean PM2.5 emission factor (EF) of traditional stoves in Kullu during baseline was 8.1 g/kg, approximately 40% higher than follow-up-1 (4.8 g/kg). Like PM2.5-EF, OC-EF was higher (~40 %) during baseline than follow-up-1 in Kullu. This suggests not only that PM2.5 mass was dominated by the organic fraction but also that OC variability dominates the seasonality in EFs. Significantly higher PM2.5 and CO EFs were observed for traditional stoves in Kullu (>20%; $p<0.05$) than Koppal during baseline, suggesting substantial inter-location variability in EFs. Among the alternative biomass stoves, the Envirofit had significantly lower CO-EF (14%; $p<0.05$) relative to traditional stoves in Koppal. However, Himansu Tandoor (improved chimney heating stove) had similar pollutant EFs to traditional stoves in Kullu. LPG had the lowest pollutant EFs, although mean CO-EF was around two times higher compared to lab values in literature, suggesting substantial variability in stove performance. Moderately strong correlation (r2=0.60) between gravimetric PM2.5 concentrations and particle scattering coefficients suggests that optical scattering data can be used as a reasonable proxy for PM2.5 mass. Single scattering albedo was somewhat negatively correlated (r2=0.15) with modified combustion efficiency but more strongly (r2=0.39) with elemental carbon to total carbon ratio (EC/TC), indicating that greater black carbon production was associated with efficient combustion. Preliminary analysis of real-time particle optical properties shows that light scattering particles were emitted more during low MCE events from traditional stoves (without chimney) compared to traditional tandoor stoves (with chimney). Second follow up data are being analyzed, and the seasonality, inter-site variability and the influence of real-time activity on emissions and particle optical properties will be explored using this extensive data set.

12CB.6

Field Measurements of Solid-Fuel Cookstove Emissions from Uncontrolled Cooking in China, Honduras, Uganda, and India. ROSE EILENBERG, Kelsey Bilsback, Michael Johnson, Jack Kodros, Eric Lipsky, Christian L'Orange, Jeffrey R. Pierce, R. Subramanian, John Volckens, Allen Robinson, *Carnegie Mellon University*

Roughly 40% of the global population relies on cookstoves for their daily cooking and heating. The impacts of cookstoves are wide-reaching, affecting human health, local air quality, and the climate; however, the magnitudes of these effects are poorly quantified. Emissions factors, which are used in both climate and health-effects models, are highly uncertain because current laboratory testing protocols do not capture the magnitude and variability of real-world emissions. Several field studies have reported in-use emissions; however, comparing the emissions between regions is difficult due to the range of reported pollutants, metrics, and study instrumentation.

To address this gap, we used a portable emissions sampler to measure in-use cookstoves in 40 households in China, Honduras, Uganda, and India. These regions covered a range of fuels, cooking practices, and stove technologies (including traditional and improved stoves). The same instruments and protocols were used at each field site. We report test-integrated fuel-based emission factors (EF), including carbon monoxide (CO), fine particulate matter (PM2.5), organic matter (OM), elemental carbon (EC), OC:EC ratios, and total particle number (PN), as well as average particle number size distributions.

Our results indicate that the characteristics of cookstoves emissions vary across regions. We found the largest PM2.5 mass EFs in China, which included some very high emitters (>100 g/kg-fuel). The smallest PM2.5 mass EFs were measured from charcoal stoves in Uganda. The magnitude of PM2.5 mass EFs in Honduras and India were similar, but their composition was distinct: the OC:EC ratios measured for stoves in India were smaller than those in Honduras, indicating that, in addition to fuel, stove technology and cooking practices impact emissions. Variations in CO EFs reflect differences in combustion conditions: smoldering operations emitting more CO emissions (as in China, Honduras, and Uganda) while flaming combustion produces less (as in India). While CO has been proposed as a proxy from PM, we did not find any correlation between average CO emissions and test-integrated PM2.5 mass overall, though there was some correlation (R2=0.67) between the average CO EFs and OM EFs for wood stoves. We did not find any statistically significant differences between the emissions of wood-burning improved and traditional stoves in Honduras and India.

A novel aspect of this study was the measurement of particle number size distributions from the field. Charcoal stoves in Uganda emitted the smallest particles with a mode near 35 nm, followed by Honduras (~40 nm), and India (~90 nm). There were a wide range in China, with three groups: one around 50 nm, one near 125 nm, and a third, broader group which appears bimodal. The total PN EFs varied by two orders of magnitude, on average. The PN EFs were lowest in India, an order of magnitude larger in Uganda, and two orders of magnitude larger in China.

Time-resolved data includes black carbon (BC), particle number, and gases (from which modified combustion efficiency, MCE, was calculated). We saw the widest and most skewed distribution of MCE and particle size in China, with stoves producing larger particles than were measured in the other countries. Stoves in India operated in the narrowest range of MCEs and emitted particle size. The distributions in Uganda and Honduras were similar. The distribution of BC and PN EFs were skewed, indicating that total emissions are driven by high emission events; elevated emissions of BC and particle number were associated with cooking events such as fire starting and fuel addition. CO emissions, however, were relatively evenly distributed across the entire test.

12CB.7

Characterizing Emissions from Diverse Domestic Biofuel Uses in Rural Malawi. ASHLEY BITTNER, Eric Lipsky, Mohammad Maksimul Islam, Andrew Grieshop, *North Carolina State University*

Malawi is a low-income, energy-poor rural country in Southern Africa, where only ~7% of the population has electricity grid access. Consequently, the majority of household energy is provided by biofuel use, i.e. collected firewood and/or charcoal. Many of the common emission sources in Malawi and their respective emission factors are uncharacterized and unquantified, limiting understanding of air quality trends and impeding evaluation via atmospheric models. As an initial step, we identify various, diverse small-scale biomass burning activities (cooking/heating/bathing, charcoal making, brick burning, whiskey distillation, etc.) for emission characterization. We conduct village-level emission sampling using a portable Stove Emission Measurement System (STEMS). The STEMS measurement system records real-time measurements of carbon monoxide (CO), carbon dioxide (CO_2), particulate matter (PM) scattering, black carbon (BC) absorption and integrated measurements of PM and organic carbon/elemental carbon (OC/EC).

In summer 2017, we monitored 2 charcoal ovens, 3 whiskey distillation events, and 20 cooking events [13 three-stone fires (TSF) and 7 improved clay cookstoves (ICS)]. We used the partial emissions capture approach for concentration measurements and the carbon balance method to estimate pollutant emission factors (EFs). Preliminary analysis of all cooking events shows an average CO EF of 104 g kg^{-1} and an average $PM_{2.5}$ EF of 13 g kg^{-1} (calculated from Teflon filter measurements). On average, the improved cookstoves had lower CO and $PM_{2.5}$ EFs (99 g kg^{-1} and 10 g kg^{-1}, respectively) compared to traditional cookstoves (138 g kg^{-1} and 15 g kg^{-1} respectively). The cookstove pollutant EFs measured in this study are comparable to those measured in previous studies. Compared to the cooking events, CO EFs associated with charcoal making and whiskey distillation were considerably higher, 240 g kg^{-1} and 142 g kg^{-1} respectively. Charcoal making had the lowest measured $PM_{2.5}$ EF (9 g kg^{-1}), while whiskey distillation had the highest measured $PM_{2.5}$ EF (19 g kg^{-1}). Preliminary analysis of the real-time PM data suggests a similar average PM scattering EF for charcoal making and whiskey distillation (19 m^2 kg^{-1} and 17 m^2 kg^{-1}, respectively). For comparison, the average PM scattering EF for the cooking events was slightly lower (14 m^2 kg^{-1}). The PM mass scattering cross-section (MSC) for charcoal was the highest (3.2 m^2 g^{-1}), and was found to be similar for whiskey distillation and cooking (1.0 m^2 g^{-1} and 0.9 m^2 g^{-1}, respectively).

For future work, we will readdress the carbon balance assumptions, particularly for the less-studied emissions from charcoal making, and we will complete analysis of the remaining data collected during summer 2017 (BC absorption, OC/EC, modified combustion efficiency, etc.). In summer 2018, in addition to another round of emission sampling, we plan to use low-cost, low-power sensor packages (AriSense, Aerodyne Research) to conduct 'fenceline' monitoring of near-source, ambient conditions for comparison with the point source measurements made with the STEMS as an initial approach to characterization of biofuel burning emissions in Malawi.

12CB.8

Interpreting Emissions from Biomass Cookstoves and Wood Stoves Using a Simple Pyrolysis Model. Christina Andersen, Robert Lindgren, Ricardo Carvalho, Vilhelm B. Malmborg, Erik Ahlberg, Natxo Garcia-López, John Falk, Axel C. Eriksson, Thomas Kristensen, Birgitta Svenningson, Christoffer Boman, JOAKIM PAGELS, *Lund University, Sweden*

Air pollution poses a challenge to both health and climate. In the developing world, 3 billion people use solid fuels for cooking in traditional open fires and stoves, which are major contributors to household and ambient air pollution (Landrigan et al., 2017). However, detailed particle emission characteristics are missing for these types of stoves.

As part of The Salutary Umeå STudy of Aerosols IN biomass cookstove Emissions (SUSTAINE), cookstoves of different technological advancement; a 3-stone fire, a rocket stove (both using wood sticks), and a natural draft (ND) gasifier stove (using wood pellets), were tested using an adjusted procedure of the standardised water boiling test. The wood sticks were from agroforestry cultivated energy wood in Kenya, while the pellet fuel was based on typical Nordic softwood (pine and spruce).

We performed highly time-resolved analysis of transient emissions. Additionally, full batch emissions were transferred to a 15 m^3 stainless steel chamber to investigate the impacts of atmospheric aging by passing the aerosol through an oxidation flow reactor (PAM [OH] ~ 1×10^8 molecules cm^{-3} h^{-1}). A SP-AMS was used to measure the non-refractory and refractory particle composition including particle phase PAHs. A seven wavelength aethalometer was used to derive equivalent black carbon (eBC) mass concentrations. Major combustion gases were measured with on-line FTIR spectroscopy. Emission factors (EF; in units mg/MJfuel) were calculated on the basis of AMS, aethalometer and CO2 measurements. The emissions were compared to emissions characterised from a conventional Nordic wood stove for domestic heating (Nielsen et al., 2017).

The emissions were interpreted in a framework of basic knowledge from wood pyrolysis (Milne 1989), where the temperature in the fuel gases is a controlling variable. The results show that the least advanced cookstoves (the 3-stone fire and the rocket stove) are associated with the highest emissions of primary organic aerosol (POA), dominated by anhydrous sugars and methoxy phenols in the particle phase and moderate emissions of benzene, toluene and xylene (BTX) in the gas-phase relative to POA. We interpret this as a result of lower effective pyrolysis and fuel gas temperature, compared to the combustion conditions in the more advanced stove. More specifically, the PM emission factor was reduced and the rBC/OA ratio was higher for the Rocket stove compared to the 3-stone fire. Furthermore, the ND pellet-fired cookstove showed even more reduced POA and PM1 mass emissions but high emissions of BTX relative to POA and genotoxic compounds such as 5-7-ring PAHs. This led to higher OA enhancements upon processing compared to the less advanced stoves. These observations are consistent with what can be expected by an increased effective pyrolysis temperature.

The conventional Nordic wood stove operated at nominal burn (NB) rate had the overall lowest emissions of POA, BTX, PAHs and SOA. This is also consistent with what can be expected by a higher combustion temperature in the heating stove, compared to the cookstoves. When operated at high burn rates, strongly increased BTX and PAH emissions were found (Nielsen et al. 2017), which explains very high OA enhancements (factor ~10 increase in OA upon aging), presumably explained by a reduced pyrolysis temperature compared to NB. The rBC emissions were still rather high for the wood heating stove, which we hypothesize was due to inefficient soot oxidation (removal) processes.

In conclusion, clear differences in PM1 emission factors of rBC, POA and SOA precursors were seen from different biomass cookstoves and one conventional wood stove for domestic heating. We suggest this could be interpreted by previously defined fundamental knowledge of wood pyrolysis.

12IM.1

A New Tandem Differential Mobility Analyzer Inversion Routine That Allows Sampling of the Entire Size Distribution in Hygroscopicity Experiments. CHRISTOPHER OXFORD, Brent Williams, *Washington University in St. Louis*

Tandem Differential Mobility Analyzers (TDMAs) can be used to determine growth factors of aerosols in high relative humidity (90%) environments. Previous TDMA inversion routines assume that the all particles measured by the TDMA are singly charged[1,2]. This assumption is valid when sampling at diameters larger than the mean of the log-normal size distribution (μ)[3]. If particles smaller than μ are sampled, the selected aerosol population can be dominated by multi-charged particles. This selection could lead investigators to improper conclusions.

In high growth factor experiments, the total TDMA instrument response can be manipulated by multi-charged particles. For hygroscopicity experiments, the final diameter of multiply-charged particles has a different mobility than their singly charged counterparts. The difference in each population's mobility will alter the total measured TDMA response. This alteration is exacerbated when sampling diameters are smaller than μ in high growth factor experiments. μ during chamber studies can often exceed 150 nm, and the upper measurement limit of many TDMAs prevent determination of the final diameter of high growth particles larger than a dry diameter of 200 nm. To sample diameters smaller than μ, the size distribution must be considered during inversion.

We created a hygroscopicity inversion routine that includes the original size distribution as an input. We calculate the number of multi-charged particles and assume that all particles sampled have the same growth factor distribution. This inversion routine improves interpretation of TDMA hygroscopicity results and allows analysis of particles across the entire size distribution.

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12IM.2

Automated Raman Spectroscopy of Ambient and Laboratory-generated Aerosols. DAVID DOUGHTY, Steven Hill, *US Army Research Lab*

We use a semi-continuous aerosol Raman spectrometer to take Raman images of particles in desert and semi-urban environments. Raman spectroscopy can be used to provide single-particle compositional information of crustal dusts, soot, and other types of aerosol particles. We focus here on the techniques to process hyperspectral Raman data, discussing fluorescence removal, cosmic ray detection, background subtraction, and the influence that choices in technique have on clustering and analysis of large quantities of Raman spectra. We also show how use of replicates can aid in automated detection of burned particles. We used machine-learning-based library matching techniques to aid in analysis of Raman spectra. Temporally resolved single-particle Raman spectra included spectra having features characteristic of sodium nitrate, humic like substances/soot, gypsum, and oxalate. Measurements made on the Jornada Experimental Range in New Mexico also exhibited spectral features consistent with as hematite, calcite, gypsum, and quartz.

12IM.3

Developing a Large Surrogate Surface to Measure Dry Deposition of Atmospheric Aerosols. ALEXANDER JOHNSON, Cliff Davidson, *Syracuse University*

Dry deposition of aerosols is a major input to urban and environmental systems and degrades natural surfaces as well as surfaces of infrastructure; surrogate surfaces are frequently used to measure dry deposition fluxes. Some of these surfaces are designed to minimize atmospheric turbulence near the leading edge and create a thin boundary layer of approximately constant thickness over the surface. These characteristics enable estimates of the lower limit of the dry deposition flux to rougher, more complex natural surfaces.

Typical collector geometries include the symmetric knife-edge surrogate surface and the frisbee-shaped surrogate surface- the latter is in the shape of an airfoil. An issue with many of these collectors is the small surface area; it is difficult to obtain reliable measurements during short dry periods, such as one, two, or three days of exposure. One category of aerosol species of interest is trace elements, but measuring deposition of trace elements can be especially difficult with small surrogate surfaces. It is often not possible to achieve a signal-to-noise ratio above unity; it is also easy to contaminate and invalidate a sample. Longer exposure times may be needed to minimize these issues, which may not be possible in climates with frequent precipitation. Therefore, there is interest in using larger surrogate surfaces to estimate dry deposition fluxes over short exposure periods.

Flat horizontal disks, 1.2 meters in diameter, were designed and used to obtain estimates of the dry deposition flux for three chemical species: sulfate, nitrate, and fluoride. The study had three objectives: to obtain a range of fluxes for each chemical species to determine if measurements were reproducible; to compare flux estimates onto the disks and onto airfoils to determine if the former can be used to estimate the lower limit of the flux to complex surfaces; and to model the boundary layer over the disks to compare with that over the airfoils.

Experiments lasting 2-6 days were conducted on the Syracuse University campus during 2016-2017. Fluxes of sulfate ranged from 71-180 μg m^{-2} day^{-1}, fluxes of nitrate ranged from 120-250 μg m^{-2} day^{-1}, and fluxes of fluoride ranged from 0.89-5.3 μg m^{-2} day^{-1}: a value in each range is an average of the two measurements from both disks. Deposition velocities of sulfate ranged from 0.11-0.75 cm/s, deposition velocities of nitrate ranged from 0.20-1.1 cm/s, and deposition velocities of fluoride ranged from 4.2-5.9 cm/s. Signal-to-noise ratios were greater than 5 for these chemical species for most experiments. Fluxes onto the airfoils were simultaneously measured for sulfate and nitrate. The ratio of the average flux onto the disks and the average flux onto the airfoils was 0.79 for sulfate and was 0.60 for nitrate; fluxes were lower onto the disks. ANSYS FLUENT was used to model the boundary layer over the disks under laminar flow for three wind speeds: 50, 100, and 500 cm/s. The boundary layer grew in thickness with distance from the stagnation point. For all wind speeds, the boundary layer was generally thicker over the disks than over the airfoils; the airfoils were modeled in a previous study. These observations suggest that there is more resistance to deposition of submicron particles onto the disks, and hence the disks can be used to estimate a lower limit to dry deposition fluxes onto complex surfaces. Experiments with disks are underway to examine the dry deposition of other chemical species with very small concentrations, which would not be possible with the airfoils or other small surfaces.

12IM.4

High Speed Imaging of Rayleigh Breakup of Charged Droplets Levitated in an Electrodynamic Balance. Mohit Singh, Neha Gawande, Y.S. MAYYA, R.M. Thaokar, *Indian Institute of Technology Bombay*

Electrospray is a well-known method for production of aerosols of nanometer size for various applications. These involve drug nanoparticle generation, coating, agricultural and automotive sprays, ink-jet printers, spray-cooling of hot surfaces, plasma coating, ion mass spectroscopy etc. An important question pertains to the Rayleigh break-up mechanisms which is responsible for the transformation of the micro-meter sized droplets ejected from the Taylor cone into nano-sized particles, as observed with instruments such as scanning mobility particle sizers. Specific question pertains to the estimate of charge and mass losses per fission. However, being a fast process, it is nearly impossible to carry out controlled observations of break-up process in electrospray itself and hence alternative tools facilitating careful observations are required. In order to accomplish this task, an electrodynamic balance in which charged droplets are levitated stably for long periods of time has been developed (Singh et al. 2017). It is made up of copper based hemispherical end-cap electrodes and circular ring electrode, connected to a AC power supply. Being large in size, it leaves sufficient gaps for inserting various observational tools such as laser beam, droplet injection needle, fibre-optics arrangement connected to PMT and low/ high speed camera. The PMT arrangement records the laser light scattered by the droplet and provide continuous signal indicating the positional and the surface stability state of the droplet. When the surface becomes unstable just prior to the Rayleigh break-up, it triggers the high speed camera for recording the emitted jet/satellite droplets. The charge is established by changing the AC frequency until the droplet becomes positionally unstable (Mathieu instability). The quantitative observations have been made on the droplets of about 70 to 200 µm, carrying charges about 15% of their respective Rayleigh charges. As the droplet undergoes evaporation, the droplet size decreases increasing the fissility to that corresponding to the Rayleigh limit, and it is observed that finally the droplet breaks up in a succession of multiple ejections. All the successive events of droplet oscillations, deformation, breakup and relaxation of drop after ejection have been captured by high speed camera connected with stereo-zoom at 130-220k fps. The experiments yield loss of about 29-40% of its original charge and 2 to 3 % of its original mass, having jet diameter of 2 to 6 µm. It has also been possible to study the dynamics of many drop levitation, their interaction and pattern formation, using the Electrodynamic balance. The presentation will discuss, the quantification of these data along with the results of numerical simulations.

Reference:

Mohit Singh, Y.S Mayya, Jitendra Gaware and Rochish M. Thaokar: J. Appl. Phys. 121, Art.No. 054503, (2017).

12IM.5

Development of an in Vitro Exposure System Enabled to Track Biological Impacts of Aerosol on Human Lung Cells in Real-Time. NIMA AFSHAR-MOHAJER, Lakshmana Chandrala, Kristine Nishida, Venkataramana Sidhaye, Joseph Katz, Kirsten Koehler, *Johns Hopkins School of Public Health*

In vitro exposure systems for studying aerosol-lung cells interactions have the limitations of inability of tracking the effects in real-time, non-uniform dose delivery onto the cell layer and being expensive. With the goal of addressing these shortcomings, we developed a novel in vitro exposure system, which simulates exposure of human bronchial epithelial cells to aerosols. We assessed the physical and biological performances of the system in comparison to a 3-well-insert stainless steel VitroCell® exposure system (VitroCell Inc., Germany) using cigarette smoke as a challenge aerosol. Then, a microscopy system was incorporated to allow visualization of the lung cells when exposed to crude oil and polystyrene latex droplets, which possess fluorescent properties. The imaging system consisted of a 20× long-distance objective, a tube lens, and a camera illustrated alterations in the ciliary beat frequency and spatial distribution of the depositing particles throughout the aerosol exposure. During exposure, live fluorescent stains were used to tag the live cells to determine cell viability. Based on the gravimetric analysis results, the average mass of the collected particles using our system versus VitroCell® were 0.177±0.027 vs 0.172±0.025 µg when exposed to 32 puffs, with a total volume of 35 mL at an incoming flow rate of 0.2 L/min per insert. Our exposure system provided a more uniform cellular exposure when exposed to the cigarette smoke. Toxicity assessment demonstrated 30% reduction in trans-epithelial electrical resistance of the exposed cells in our system compared to 8% reduction when VitroCell® was used. The percentage change in permeability of the cells monolayer after exposure to the cigarette smoke was 195% vs 175%.

We observed a more uniform delivery in our proposed exposure system at a much lower cost. Our system also facilitates the live visualization of cells during the exposure and allows an investigation of the changes within the epithelium to disrupt tissue integrity in response to inhalation of aerosols.

12IM.6

Rapid Measurement of Sub-micrometer Aerosol Size Distribution Using a Fast Integrated Mobility Spectrometer.

YANG WANG, Tamara Pinterich, Jian Wang, *Brookhaven National Laboratory*

Rapid measurement of sub-micrometer particle size distributions enables the characterization of aerosols with fast changing properties, and is often necessary for measurements onboard mobile platforms (e.g., research aircraft). Aerosol mobility size distribution is commonly measured by a scanning mobility particle sizer (SMPS), which relies on voltage scanning or stepping to classify particles of different sizes, and may take up to several minutes to obtain a complete size spectrum of aerosol particles. The recently developed fast integrated mobility spectrometer (FIMS) with enhanced dynamic size range classifies and detects particles from 10 to ~ 600 nm simultaneously, allowing sub-micrometer aerosol mobility size distributions to be captured at a time resolution of 1 second. The FIMS consists of a parallel plate mobility separator, a condenser, and a CCD camera. Inside the separator, an electric field separates charged particles based on their electrical mobilities. The spatially separated particles then pass through a condenser, where particles as small as 7 nm grow to above 1 µm through water or heptanol condensation. Finally, the grown particles are illuminated by a laser sheet and imaged onto a CCD array. The images provide both aerosol concentration and position, which directly relate to the aerosol size distribution.

In this study, we present a detailed data inversion routine for deriving aerosol size distributions from FIMS measurements. The inversion routine takes into consideration the FIMS transfer function, particle penetration efficiency in the FIMS, and multiple charging of aerosols. The accuracy of the FIMS measurement is demonstrated by comparing parallel FIMS and SMPS measurements of stable aerosols with a wide range of size spectrum shapes, including ambient aerosols and aerosols classified by a differential mobility analyzer (DMA). The FIMS and SMPS-derived size distributions agree well for all aerosols tested, showing differences within 5% in average particle size and total number concentration. In addition, total number concentrations of ambient aerosols were integrated from 1 Hz FIMS size distributions, and compared with those directly measured by a condensation particle counter (CPC) operated in parallel. The integrated and measured total particle concentrations agree well within 5%.

12IM.7

Uniformity of Particle Concentration after Mixing Aerosol Flows. David Walker, Tyler J. Johnson, Robert Nishida, JONATHAN SYMONDS, Kingsley Reavell, *Cambustion*

Aerosol experiments are frequently performed with low flow Reynolds numbers (Re<4000), and it is often necessary to mix two streams (for example an aerosol flow with clean make-up air), then later divide the mixed stream between different instruments. It is important that the combined stream is uniformly mixed before the division occurs, otherwise the concentration in the two substreams may be significantly different.

In this work, the variation in aerosol concentration across the cross section of a tube carrying a flow from different designs of tee mixing an aerosol flow from a nebuliser with filtered dilution air was measured by sampling from the flow through a 0.7mm capillary tube. The range of flow rates tested and the velocity profile in the sample tubes prevents true isokinetic sampling by this capillary so the experiments were performed with a NaCl aerosol of approximately 84 nm CMD (mobility diameter) to minimise artefacts from this sampling.

Two 6mm diameter tees of different geometries were tested with a 0.8 l/min aerosol + 1.2 l/min diluent flow. For a plain tee, the concentration distribution measured 30 tube diameters downstream of the mixing axis showed a 38% total concentration variation (ie. minimum to maximum) of the mean. A coaxial geometry, with the sample flow introduced into the centre of the dilution flow via a coaxial 6mm tube gave a concentration variation of 36%, not significantly different from the plain tee result.

With the length of the downstream tube increased to 400 tube diameters, the variation was reduced to 17%. Introducing a 14 element static mixer produced a 2.4% variation at the 30 tube diameter location, roughly comparable with the uncertainly of the experiment. The static mixer was additionally tested for particle losses which were found to be less than 5%.

The 6mm coaxial tee and a 10mm version were tested at higher flow rates. For the 6mm tee at 30 tube diameters, using 1.7 l/min sample and 5 l/min dilution flow, the variation was 35%; while using a 2.5 l/min sample and 20 l/min dilution flow, the variation reduced to 3.0%. The 2 l/min, 6.7 l/min and 22.5 l/min conditions correspond to Reynolds numbers of approximately 460, 2200 and 7700 respectively.

The 10mm tee measured at 30 tube diameters with 22 l/min flow produced a variation of 4.7%. Closer to the mixing point, at 6 tube diameters, the variation was higher at 15%. Flows of 32 l/min and 62 l/min produced variations of 17% and 27% respectively at that location. Reynolds numbers for the 22 l/min, 32 l/min and 62 l/min conditions were approximately 3700, 5400 and 10500 respectively.

These results suggest that mixing at typically laminar Reynolds numbers (< approximately 4000) even with long tube lengths downstream of the mixing tee is poor and that a mixing element should be used. For low flows, of the order of a litre per minute or less, it is difficult to achieve higher Reynolds numbers. For experiments performed at higher flows where turbulent Reynolds numbers can be achieved, satisfactory mixing may be achieved if tube lengths are sufficient: higher turbulent Reynolds numbers will require longer mixing lengths.

12IM.8

M-WINS Inlet for Continuous PM2.5 Sampling. THI-CUC LE, Jung-Che Sung, Krishna Kumar Shukla, Chuen-Jinn Tsai, *National Chiao Tung University*

Most of PM2.5 FRM samplers and FEM monitors use filter media to capture particles after particles are size-classified by the well impactor ninety-six (WINS) or very sharp cut cyclone (VSCC). The impaction glass fiber filter substrate (GFFS) of the WINS is coated with silicone oil to eliminate particle bounce. However, the particle loading effect occurs when a particle mound is formed on the impaction substrate after a long sampling time leading to under-sampling of PM2.5. The performance of an uncleaned VSCC was claimed not to be affected by the particle loading effect. However when the sampling period was over 5 days, we found fluctuations in measured PM2.5 concentrations as compared to the concentrations of a VSCC which was cleaned daily. Our previous work (Le and Tsai, 2017) developed a modified WINS (M-WINS) with a wetted GFFS through which a small water flow was injected upward at the center to wash off deposited particles continuously. The particle loading effect was eliminated successfully. Instead of using continuous water flow, the current study uses vacuum oil which was injected periodically to wash off the deposited particles. The laboratory test results showed that the M-WINS had a similar cut-size (2.43 ± 0.02 µm) and sharpness (1.22) as the WINS. Without cleaning the substrate, the particle loading test at the laboratory for M-WINS showed that the cut-size was decreased from 2.49 to 2.18 µm as the particle mass loading was increased from 0 to 3.5 mg with a particle mound formed on the substrate. The cut-size of M-WINS was able to recover to 2.46 µm when the oil flow was injected for just 1-min at the flow rate of 3 mL/min to wash off the mound. This saves oil consumption. The field comparison tests of the M-WINS collocated with a clean VSCC and a clean WINS is being conducted at National Chiao Tung University (NCTU), Taiwan. During the field tests, the M-WINS substrate was washed with a small amount of oil every day for just 1-min at the flow rate of 3 mL/min to keep the surface clean. The preliminary results indicate that the M-WINS has a great potential to measure PM2.5 accurately for a longer sampling period without the need of maintenance and the amount of vacuum oil consumption is very small, only 3 ml per day. In addition, the used oil can be reused after being filtered.

Keywords: PM2.5, aerosol sampling, particle bounce, particle overloading, impactor, cyclone

Reference: Thi-Cuc Le and Chuen-Jinn Tsai. 2017. Novel non-bouncing PM2.5 impactor modified from well impactor ninety-six, Aerosol Sci. Technol., Vol. 51: 1287-1295.

12LC.1

Source Apportionment of Particulate Matter Using Low-Cost Particle Sensors with Co-Located Reference Measurements. DAVID HAGAN, Jesse Kroll, Eben Cross, Joshua Apte, Shahzad Gani, Lea Hildebrandt Ruiz, Sahil Bhandari, Gazala Habib, *MIT*

The past several years has seen the emergence of many low-cost commercial devices for measuring particulate matter (PM) for the monitoring of indoor and outdoor air quality. Although the quality of data from these devices has improved as our understanding of their operation has developed, optical-based particle instruments (OPC's) suffer from sources of error that limit their value for air quality and source apportionment studies (i.e., lack of composition information, lack of measurements of the smallest particles). Often, deployments of low-cost PM sensors are done in conjunction with additional low-cost, gas-phase sensors which are typically treated as separate instruments. In this work, we present methods (based on a variant of a recurrent neural-network algorithm) for using the additional information provided by gas-phase sensors and available composition information (black carbon, PM1 composition via Aerosol Chemical Speciation Monitor) to enhance our understanding of the particle measurements and increase the utility of deploying low-cost sensor networks. We discuss these results in the context of two multi-year, outdoor sensor deployments in very different environments (Boston, Delhi). In addition, we present results on the effectiveness of using factor analysis as a tool to learn more about pollutant sources using low-cost sensor networks.

12LC.2

A Low-cost Sensor Network to Improve Air Quality Management: A Case Study in Jining, China. XIAOHUI QIAO, Qiang Zhang, Fenglin Liu, Ying Long, Jingkun Jiang, *Tsinghua University*

Severe fine particulate matter ($PM_{2.5}$) pollution along with higher mortality risk raised unprecedented public awareness in China. To realize Chinese government's urgent vision of improving air quality, more refined actions are needed. However, the spatial resolution of current air quality monitoring system is not enough to support that. The emergence of low-cost, compact PM sensors enables measurement at high spatial resolution that can provide new opportunities to couple with the existing monitoring system and to improve air quality management capability. We established a monitoring network with 161 packaged low-cost sensor platforms in Jining, a city in eastern China and with a population of ~3 million. Previously, there were only 8 standard air quality monitoring stations in Jining. The sensor network together with the standard stations helps the government both at the city level and at the township level to implement air quality management strategies. Based on the network, ranking among township can be established and be used to motivate and to guide air pollution control at the township level.

Through laboratory and field evaluation of current available $PM_{2.5}$ sensors, the PM sensor from Oneair was selected and integrated into a platform together with other sensors for gaseous species. Depending on the availability, either utility power or solar panel was used to power the platform. Data measured by the platform (including the GPS information and meteorology parameters) are transferred to the main database server through the GPRS wireless network. In this talk, data from Nov. 2016 to Feb. 2017 were taken as an example. Through comparisons with standard stations and adjacent platforms, we conclude that the network was running in good condition and the data quality are good. Based these data, air quality was assessed at the township level by ranking them from three perspectives, i.e., ambient $PM_{2.5}$ concentration, population-weighted $PM_{2.5}$ concentration, and $PM_{2.5}$ concentrations of all the platforms. Population-weighted $PM_{2.5}$ helps to take exposure into consideration. The rank among all the platforms helps to find out potential emission sources.

12LC.3

Development and Application of a New Palm-Sized Optical PM2.5 Sensor. TOMOKI NAKAYAMA, Yutaka Matsumi, *ISEE, Nagoya University*

Aerosol particles have important roles in the earth's climate and air quality. It has been recognized that fine particulate matter, such as $PM_{2.5}$, negatively impacts human health through heart disease, stroke, lung cancer and chronic obstructive pulmonary disease, and this results in the premature mortality of many people. The $PM_{2.5}$ is expected to be heterogeneously distributed in both indoor and outdoor atmospheres because of its many direct emission sources and secondary formation processes. High-density multipoint observations are needed to understand the source, transport, and sink of $PM_{2.5}$ and its effects on climate, air quality, and human health. The development and application of a low-cost palm-sized $PM_{2.5}$ sensor, which can measure $PM_{2.5}$ mass concentrations precisely and accurately, is important to achieve high-density multi-point observations. A palm-sized $PM_{2.5}$ sensor with low power consumption and high temporal resolution can also be applied to mobile measurements for personal exposure studies and to airborne measurements using balloon sonde and unmanned aircraft.

We have developed a new palm-sized optical $PM_{2.5}$ sensor with Panasonic cooperation. The $PM_{2.5}$ mass concentration was calculated from the distribution of light scattering intensity by considering relationship between scattering intensity and particle size. The results of laboratory tests suggested that the sensor can detect particles with diameters as small as ~0.3 µm. The performance of the $PM_{2.5}$ sensor was evaluated by comparing the obtained data with corresponding data from large beta-attenuation monitor (BAM) instruments in many places. As results, good agreement between our $PM_{2.5}$ sensor and BAM instrument was observed. This sensor has been applied to the observation in eight Asian countries. We have also developed a personal exposure measurement system, consisting of the $PM_{2.5}$ sensor and a smartphone. The obtained $PM_{2.5}$ and GPS position data are automatically transferred to a cloud server. We are planning to apply this system to personal exposure monitoring studies in developing countries.

Reference

T. Nakayama, Y. Matsumi, K. Kawahito, and Y. Watabe, Development and evaluation of a palm-sized optical $PM_{2.5}$ sensor, Aerosol Sci. Technol., 52, 2-12 (2018).

12LC.4

Spatial and Temporal Variability of Air Quality in Pittsburgh, Pennsylvania with a 50-Node RAMP Network. R. SUBRAMANIAN, Carl Malings, Rebecca Tanzer, Aliaksei Hauryliuk, Provat Saha, Aja Ellis, Rose Eilenberg, Sriniwasa P.N. Kumar, Naomi Zimmerman, Allen Robinson, Albert A. Presto, *Carnegie Mellon University*

Low-cost sensors have enabled 24x7 continuous air quality monitoring with high spatial resolution, though the data is often associated with large uncertainties. The Real-time Affordable Multi-Pollutant (RAMP) monitor, developed at Carnegie Mellon University in collaboration with SenSevere (Pittsburgh, PA), can measure up to four gases out of carbon monoxide (CO), sulfur dioxide (SO_2), nitric oxide (NO), nitrogen dioxide (NO_2), ozone (O_3), and volatile organic compounds (VOCs), along with carbon dioxide (CO_2), temperature, and relative humidity. Calibration models based on periodic collocations with reference monitors and machine learning algorithms have enabled the RAMP to meet EPA's supplemental monitoring (CO, O_3) or hot spot (NO_2) data quality. SO_2 performance is also promising at tens of ppb or higher. The RAMP uses either a Met-One Neighborhood PM monitor or a PurpleAir PM sensor to measure fine particulate mass ($PM_{2.5}$). The PM data is corrected for humidity effects using an aerosol hygroscopic growth model and an average aerosol composition for Pittsburgh based on aerosol mass spectrometry data. A final correction is applied based on long-term collocation of one RAMP with a local regulatory monitor to account for Pittsburgh-specific aerosol size distributions that may be different from the factory calibration.

A network of fifty RAMP sensors has been deployed in and around the city of Pittsburgh, Pennsylvania since Summer 2017, representing (to our knowledge) the largest long-term deployment of multipollutant sensor systems. The RAMPs are hosted by schools, residences, public facilities, businesses, and religious establishments. Locations identified by land-use attributes (traffic, restaurant density, and building height) were obtained through direct contact or with the help of local community organizations and interested individuals.

The 50-RAMP network allows us to examine the spatial and temporal variability of air quality across a major urban area at an unprecedented scale. Elevated levels of CO and $PM_{2.5}$ were observed in the residential East End of Pittsburgh, which is home to several schools and restaurants, with arterial roads running through it and connecting to a major highway, because of which vehicular traffic can exhibit sharp diurnal patterns. CO variability in some of these locations – particularly at some schools – was relatively high, with long-term standard deviation in CO between 300-400 ppb. Sites in downtown Pittsburgh, which has heavy traffic during the day and is bordered by several highways, showed long-term CO standard deviations below 150 ppb. This could be because while average CO during Summer 2017 in the East End locations were comparable to that in downtown Pittsburgh (300-400 ppb), CO was higher in the East End the following Winter.

$PM_{2.5}$ averages varied from 7.7-11.6 $\mu g/m^3$ across the RAMP network. While the highest $PM_{2.5}$ concentrations were recorded in the Monongahela Valley (home to coke plants and a steel mill), similar concentrations (about 2 $\mu g/m^3$ higher than the nearest regulatory monitor) were observed in the Homewood neighborhood, an environmental justice area within city limits. The lowest $PM_{2.5}$ concentrations were observed in the suburban neighborhoods of Fox Chapel, Aspinwall, and Mt Lebanon– but also in the near-downtown, poorer Hill District neighborhood. Winter-time $PM_{2.5}$ is higher than summer concentrations in the river valleys by about 3 $\mu g/m^3$, but the exact opposite is true for the relatively elevated East End locations; either shift is about 30% of the city-wide average $PM_{2.5}$. NO_2 levels vary by as much as ±3 ppb across the RAMP network, though a pattern is not readily evident and needs further investigation. Additional detailed analysis and insights from the RAMP network with learnings for future low-cost sensor networks will be presented.

12LC.5

City Wide Mobile Air Sensor Network (MASEN) in Hong Kong for Evidence Based Air Quality Management. ZHI NING, Fenhuan Yang, Dane Westerdahl, *City University of Hong Kong*

In urban areas, vehicles emissions are a major source of air pollution (HEI, 2010), especially particulate matter (PM) and nitrogen oxides (NOx). This study presents the recent work in Hong Kong using mobile air sensors on buses to form a large scale sensor network with continuous measurements of PM2.5, NO, NO2, CO and CO2 pollutants along more than 40 bus routes. We have found high heterogeneity of the pollutants concentrations in more complex urban terrain with its complexity in built environment, which poses an increasing challenge to accurately quantify and assess trend of air pollution for science based evidence collection for policy making. The mobile sensor network data also showed interesting effect of combined impact of local and regional pollutions. This also leads to increasing consideration and discussions for a new monitoring paradigm shift from static ambient monitoring to spatio-temporally resolved higher density monitoring network. Recent technological advances in air monitoring allow unprecedented opportunities for such air monitoring network using low cost and high quality sensors, which require less infrastructure support than the traditional stationary monitoring stations. New sensing techniques in dense and complex urban environments can be operated at a fraction of the cost of conventional devices and produces unprecedented “big data” in high temporal and spatial resolution. Such mobile network would also have high potential to supplement the existing regulatory air monitoring networks, and provide evidence of association between the roadway network traffic and the air quality in different urban areas.

12LC.6

Long-term Performance Evaluation of Commercial Low-Cost PM2.5 Sensors in Houston, Texas. H. LANGLEY DEWITT, Bradley Flowers, Will Ollison, Walt Crow, *American Petroleum Institute*

Advances in air pollution monitoring technologies have enabled the development and proliferation of low-cost and portable air pollution sensors, which can monitor a variety of gas-phase and particulate matter (PM) species. Because of their lower cost, these air quality sensors are more accessible to researchers and the public, enabling collection of air quality data at significantly higher spatial and temporal resolution. As the use of low-cost air quality sensors has increased in recent years, laboratory and field performance evaluations have increasingly been conducted to quantify the quality of data obtained in comparison to EPA federal reference methods and research grade instrumentation. However, many of these sensor evaluations have been short-term; ranging from one week to several months in duration. There remains a need to demonstrate the quality of low-cost sensor data over much longer time periods, which would be more representative of standard usage.

This presentation will focus on the results of a 10-month study conducted by the American Petroleum Institute (API) to examine the long-term performance attributes of two low-cost optical particle counters, a Dylos Model DC1100 and an AirBeam. Field-testing was performed continuously from March 1, 2017 through December 31, 2017 in Houston, TX at an ambient air monitoring station operated by the Houston Regional Monitoring (HRM) network. This site was chosen due to its proximity to the Houston Industrial Complex and the complex nature of emissions sources in Houston. The site experiences wide ranges of temperature and humidity to further evaluate sensor performance under different meteorological parameters. Factory installed and post measurement algorithms for converting optical particle counts to PM2.5 mass concentrations were tested. The results from the low-cost PM2.5 sensors are directly compared with paired continuously operating Met One Model 1020 PM2.5 Beta Attenuation Federal Equivalent Method (FEM) Monitors and a Met One Super SASS PM2.5 chemical speciation sampler. The results from this study highlight the importance of post-processing on the fidelity of low-cost PM2.5 sensor data and potential issues with longer-term deployments, which to our knowledge have not been addressed with previous field campaigns.

12LC.7

A Community Network of 100 Low-Cost Black Carbon Sensors. CHELSEA V. PREBLE, Julien Caubel, Troy Cados, Joshua Apte, Thomas W. Kirchstetter, *University of California, Berkeley*

We developed a low-cost black carbon (BC) sensor that employs the filter-based light transmission method and field tested it to verify good precision and correspondence with current commercial black carbon instruments. We built over 100 of these BC sensors and deployed them as a connected air quality network in West Oakland, California. West Oakland is a mixed residential and industrial community that is adjacent to regional port and rail yard facilities and surrounded by major freeways. As such, the community is affected by diesel particulate matter emissions from heavy-duty diesel trucks, locomotives, and ships associated with freight movement.

In partnership with the Environmental Defense Fund, Bay Area Air Quality Management District, and West Oakland Environmental Indicators Project, we positioned the BC sensors outside of residences and businesses, along truck routes and arterial streets, along the Port of Oakland boundary, and at upwind locations. We operated this air quality network for 100 days beginning mid-May 2017.

Throughout the 100-day period, each of the 100 sensors transmitted data via a cellular network. A MySQL database was built to receive and manage the data in real-time. The database included diagnostic features to monitor each sensor's operational status and facilitate the maintenance of the network.

Spatial and temporal patterns in black carbon concentrations in West Oakland are observed to be driven by truck activity within the community. “Hot spots” exist along truck routes, near trucking facilities, and around businesses that use trucks to transport goods and materials. Almost everywhere, BC concentrations are higher on week-days than weekend-days, as is truck activity. The community-average black carbon concentration matches well the concentration measured at a centrally located site operated by the Bay Area Air Quality Management District. However, on average, 75% of locations within the community are more polluted than the centrally located monitoring site, with daytime average BC up to 1.75x higher. Daytime average concentrations along the Port of Oakland boundary and designated truck routes around the community are up to 3x higher than the central monitoring site average. Overnight, the spatial gradient within the West Oakland neighborhood diminishes, such that BC concentrations are more uniform. Areas downwind of the freeway, along the Port of Oakland boundary, and at some trucking facilities have persistent elevated BC concentrations in the evening and early morning hours.

12LC.8

Cloud-based Application to Manage Data from Distributed Air Quality Sensors Networks. BRANDON FEENSTRA, Ross Cheung, Vasileios Papapostolou, Andrea Polidori, *South Coast Air Quality Management District*

Distributed networks of small air quality sensors are now a reality. Technological advances in low-cost aerosol and gas pollutant sensors have provided the opportunity to build large networks of sensors to measure concentrations of air pollutants. In one year, a single air quality sensor can generate more than 2 million measurements, requiring time changes, time averaging, time matching, joining, validations, and calibrations. Environmental air quality projects quickly become a data science and/or computer science project with a new set of challenges in data storage and analysis. Establishing networks of sensors requires a significant investment in new infrastructures to handle the data load. The South Coast Air Quality Management District (SCAQMD) is poised to deploy over 500 low-cost sensors by end of 2018. To meet the needs of this oncoming data generation, the SCAQMD has started building a reliable and scalable cloud-based platform to ingest, persist, analyze, and visualize substantial quantities of air quality monitoring data. We will present an approach to go from Internet-of-Things (IoT) connected air quality sensors to an online data dashboard for public consumption. Data work-flows and best practices will be discussed along with data validation and sensor calibrations.

12MG.1

Challenges of Air Quality Monitoring and Forecasting in Different Mega City Environments. G. BEIG, *IITM, Pune, India*

The “System of Air Quality and Weather Forecasting And Research (SAFAR)” was launched in 2010 as a pilot project of GURME of WMO for Indian Metro cities. It has now been implemented in 4 metro cities, namely, Delhi, Pune, Mumbai and Ahmedabad. The SAFAR provides location specific information on air quality in near real time and its forecast along with weather information. There are 4 basic components of SAFAR: Air pollutant and weather Observational Network, Emission Inventory, Forecasting Model, and Communication to Society. The distribution of the major pollutants ozone (O_3), oxides of Nitrogen (NO_x), Carbon monoxide (CO), Benzene, PM_{10}, and $PM_{2.5}$ has been studied in detail and their forecasting skill is tested. The major challenge in Indian mega cities is particulate pollution and not the gaseous pollutants. Each city has dense observational network on 10 locations. Scientific evaluation of the data generated from AQMS and WRF-Chem provides a basis to understand the air quality status. However, each city has different challenges. While Pune’s forecast has smooth sailing, Delhi forecast is posing challenges on each passing day. The frequencies of extreme pollution events are on rise in Mega cities like Delhi and system requires vigilant eye on hourly basis. The air quality of the Bombay region is highly influenced by sea breeze being a coastal station. This paper will address issues and challenges in predicting the air quality in different microenvironments of different mega cities.

12MG.2

Contributions to Disease Burden from Major Sources of Air Pollution in India. Michael Brauer, Aaron Cohen, KATHERINE WALKER, Richard T. Burnett, Joseph Frostad, Qiao Ma, Randall V. Martin, Shuxiao Wang, Chandra Venkataraman, HEI GBD-MAPS Working Group, *Health Effects Institute*

Ambient air pollution is a leading global risk factor – with 7.5% of total deaths (4.1 million) attributable to exposure to fine particles ($PM_{2.5}$) according to the most recent Global Burden of Disease estimates (IHME GBD 2016). A majority of this burden is found in low and middle-income countries in Asia, the result of emissions from a variety of sources including the burning of coal for thermal power and industry, household burning of solid fuels, and transportation. To help identify and support priorities for air quality management efforts, the Health Effect Institute launched the Global Burden of Disease-Major Air Pollution Sources (GBD-MAPS) project to estimate both the air pollution levels and the health burden attributable to major air pollution sources. GBD MAPS was first conducted in China and the results have been presented previously; results for the Indian study are presented here.

The objective of this study was to estimate the contributions of major source sectors to ambient $PM_{2.5}$ concentrations and disease burden under current conditions and multiple future emissions scenarios for urban and rural India.

GBD-MAPS extended the GBD methodology, using emissions inventories and projections together with chemical transport model (GEOS Chem) simulations to i) estimate source contributions to ambient $PM_{2.5}$ concentrations and to population-weighted exposures ii) assess the contribution of major sources of $PM_{2.5}$ pollution to current disease burden in India (2015 base year), and iii) predict the impact of different future emissions control scenarios on air quality (2030) and resulting disease burden for both urban and rural areas of India (2050).

In India, residential biomass combustion for cooking and heating was the largest contributor to ambient $PM_{2.5}$ exposure and burden, responsible for 25% or 268,000 deaths in 2015. This source was followed in magnitude by coal combustion (15.5% or 169,000 deaths), open burning of agricultural residue (6.1% or 66,000 deaths), and a combination of sources including transport, distributed diesel, and brick production. Increases in future $PM_{2.5}$ attributable deaths were projected for all future emissions scenarios, due to aging and growing populations, but more deaths were avoided with increasingly stringent emissions scenarios.

Heavy industrial and population growth in India suggest "business as usual" scenarios to result in severe burden from air pollution from multiple sources for years to come in rural, as well as urban areas. Aggressive legislation and enforcement of air quality management are required to substantially reduce the future burden of air pollution in India.

12MG.3

Correlation between PM2.5 and Particle Number Concentrations in Four Major Cities: Toronto, Los Angeles, Helsinki and London. ALMA LORELEI DE JESUS, Md Mahmudur Rahman, Mandana Mazaheri, Luke Knibbs, Helen Thompson, Greg J. Evans, Cheol H. Jeong, Markku Kulmala, Tuukka Petäjä, Krista Luoma, Hilkka Timonen, Jarkko Niemi, Roy M. Harrison, David Beddows, Constantinos Sioutas, Mohammad Sowlat, Lidia Morawska, *Queensland University of Technology*

Gaining more knowledge on how different particulate metrics are related would help in successfully controlling particulate matter (PM) concentrations in the ambient air. This study focused on the mass and number concentrations, particularly $PM_{2.5}$ or mass concentration of particles with diameter of <2.5 µm in order to illustrate that mitigating $PM_{2.5}$ would not necessarily reduce the ultrafine particles (UFP) concentration. Particles with diameter <0.1 µm are best quantified by the particle number concentration (PNC). The two parameters, $PM_{2.5}$ and PNC are affected by different drivers, therefore may vary spatially and temporally between cities. $PM_{2.5}$ is relatively more homogenous within an air shed while PNC is more variable depending mainly on the distribution of the combustion emission sources. To better understand these two important metrics and demonstrate their similarities and differences, this study aims to provide quantitative information on the relationship between ambient $PM_{2.5}$ and PNC in four cities: Toronto, Canada; Los Angeles, USA; Helsinki, Finland; and London, UK. All these cities are located in the temperate region though Helsinki and Toronto are classified under Moist Continental Mid-Latitude Climate while London and Los Angeles are classified under Moist Subtropical Mid-Latitude climate based on the Köppen-Geiger system. Urban areas are particularly interesting because high population density implies that considerable amount of anthropogenic pollutants are produced in any city.

One-year hourly averages of $PM_{2.5}$ and PNC were acquired and analysed. Data analysis include: comparing hourly average of $PM_{2.5}$ and PNC using descriptive statistics, statistical models and non-parametric tests; and identifying the factors that drive the relationship. Our results showed that the annual median of $PM_{2.5}$ concentrations for Toronto, Helsinki and London were similar (6.6, 6.9 and 7.8 $\mu g.m^{-3}$, respectively) but Los Angeles was a bit higher at 16 $\mu g.m^{-3}$. The elevated $PM_{2.5}$ in Los Angeles was due to formation of secondary aerosols influenced by the area's meteorological characteristics according to Hasheminassab et al. (2014). London and Los Angeles had almost the same annual median of PNC (7.2 and 7.3 x 10^3 $\#.cm^{-3}$, respectively) compared to Toronto and Helsinki that were high (1.5 and 1.1 x 10^4 $\#.cm^{-3}$, respectively). This can be attributed to the monitoring site category since it was an urban background station for London and Los Angeles and a roadside station for Helsinki and Toronto; therefore, traffic was directly affecting PNC. The annual medians of both $PM_{2.5}$ and PNC were compared and statistical tests were carried out to assess significant differences between cities. The results indicate significant differences in $PM_{2.5}$ and PNC between cities.

Regardless of the difference in climate, all cities showed similar patterns in the diurnal and seasonal variations. The diurnal trend of the PNC in all cities showed traffic peaks in the morning and evening, which was not the case for $PM_{2.5}$. On the other hand, a seasonal trend was observed for both $PM_{2.5}$ and PNC where concentrations were high during cold months and lower during the warm months. Establishing the relationship between these two parameters is important to determine the more reliable parameter to be used in exposure and epidemiological studies as well as identifying the effective regulatory control measures. There were weak to moderate correlations between $PM_{2.5}$ and PNC across all cities. Therefore, both parameters must be considered in implementing regulatory control measures for ambient PM.

Reference: Hasheminassab, S., Daher, N., Saffari, A., Wang, D., Ostro, B. D., & Sioutas, C. (2014). Spatial and temporal variability of sources of ambient fine particulate matter ($PM_{2.5}$2.5) in California. *Atmospheric Chemistry and Physics,* 14(22), 12085. doi:http://dx.doi.org/10.5194/acp-14-12085-2014.

12MG.4

Characterization of Polycyclic Aromatic Hydrocarbons (PAHs) in Fine Particulate Matter (PM2.5) in Urban New York.

HAIDER A KHWAJA, Zafar Aminov, Wen Yuan, Mirza M. Hussain, Shannon Foote, *Wadsworth Center, University at Albany*

Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous environmental pollutants that are formed in combustion processes of carbonaceous materials at high temperatures. Because many of them and their analogues are strongly potent carcinogens and/ or mutagens, the occurrence and fate of PAHs in the environment is of great interest. Concentrations of PAHs adsorbed to respirable fine particulate matter ($PM_{2.5}$) were determined from two urban sites in New York viz., Botanical Gardens, New York City and Empire State Plaza, Albany. $PM_{2.5}$ samples were collected using high-volume sampler on quartz filters over 24 h sampling period. Samples were extracted using soxhlet extraction technique and analyzed by GC/MS. Total PAH concentrations at New York City and Albany ranged 275 – 2821 pg/m^3 and 259 – 2069 pg/m^3 , respectively. Concentrations of PAHs at these two urban sites are comparable to those found in Los Angeles, California. In urban areas, vehicular emissions are likely to be the primary contributor to PAH concentrations with additional local contributors like cooking fuels and industrial emissions. Among the 23 PAHs, benzo[*g,h,i*]perylene was the most abundant PAH at both sites. It contributed 11 – 23% to the sum of PAHs. The trend of the concentrations of the major PAHs found in the present study were benzo[*g,h,i*]perylene > benzo[*b*]fluoranthene > indeno[*1,2,3,c-d*] pyrene > benzo[*e*]pyrene > fluoranthene > pyrene > benzo[*a*]pyrene > phenanthrene > chrysene > benzo[*k*]fluoranthene > naphthalene. Most common PAHs (benzo[*g,h,i*]perylene, fluoranthene, pyrene, phenanthrene, and. benzo[*b*]fluoranthene are associated with diesel and gasoline exhaust particles. The large amount of benzo[*a*]pyrene in the ambient samples is likely from wood burning. Levels of seven PAH considered as possible or probable carcinogenic (benzo[*a*]anthracene, chrysene, benzo[*b*]fluoranthene, benzo[*k*]fluoranthene, benzo[*a*]pyrene, indeno[*1,2,3,c-d*]pyrene, dibenzo[*a,h*]anthracene represented a significant portion of the PAH contained in $PM_{2.5}$. Using published relative carcinogenic potency factors for individual PAH, the proportion of carcinogenic potential represented by benzo[*a*]pyrene was evaluated. Results suggest the suitability of benzo[*a*]pyrene as a marker for the carcinogenic potential of the PAH mixture in ambient air.

12MG.5

Relative Importance of Emissions from Ships, Locomotives, and Freeways in the Communities near Ports of Los Angeles and Long Beach and Their Impact on the Air Quality of Los Angeles Basin. AMIRHOSEIN MOUSAVI, Mohammad Sowlat, Sina Hasheminassab, Olga Pikelnaya, Andrea Polidori, George Ban-Weiss, Constantinos Sioutas, *University of Southern California*

In this work, the impact of emissions from different sources (ships, major freeways, locomotive railway and LAX airport) in the vicinity of port of Long Beach (POLB)(north Long Beach community) and their contribution in the local and regional scale emissions in the Los Angeles air basin is evaluated. particle number (PN), $PM_{2.5}$ mass and black carbon (BC) ship emission factors were obtained by plume analysis reported by a comprehensive study at POLB by Chalmers University in October-November 2015. In addition, freeway emission factors for the aforementioned species were calculated based on the on-road emission measurements on I-710 and I-110 freeways. Local scale emission rates were quantified with respect to the “impact zone” of POLB with the predominant southerly winds from coast to inland, considering emissions from cargo handling equipment, locomotive railway in POLB and truck activities in the port area. At the local scale, $PM_{2.5}$ emission rates were driven by locomotive and ship emissions with emission rates of 43.5±7.8 and 39.1± 12.1 kg.day^{-1}, respectively. While locomotive emissions dominated the PN emissions at the local scale, freeway PN emission rates in the impact zone with 8.72× 1019 ± 1.21×1018 particles.day^{-1} were comparable with the POLB good-movement emission rate. At the local scale, POLB vessel and cargo handling emission sources contributed to the PN, BC and PM2.5 emissions by 16±4%, 21±10% and 28±11%, respectively. Moreover, In the regional scale, PN, PM2.5 and BC total freeway emissions rates of Los Angeles County are 2.92±0.84, 5.53±1.22 and 2.34±0.76 times greater than the total local POLB emissions, respectively. Presented statistics highlight the importance of locomotive and ship emissions from POLB within the impact zone as well as regional scale.

12MG.6

Comprehensively Assessing the Drivers of Future Air Quality in California. SHUPENG ZHU, Michael MacKinnon, James V. Soukup, Donald Dabdub, *University of California, Irvine*

Future air quality, especially aerosol and ozone, will be governed by a range of factors including the physical impacts of climate change and socioeconomic factors including emission control efforts, demands in energy end-use sectors and the deployment of alternative technologies. While the impact of these factors on air quality has been studied from an individual perspective, there is a lack of information considering them from a holistic perspective, e.g., assessment of the combined impacts, comparison among factors using a consistent modeling platform, etc. Additionally, previous work has focused mostly on the national or global scale. Therefore, there is a need for comprehensive assessment of future air quality at the state level to account for the major drivers of pollutant concentrations from a holistic perspective.

In this study, air quality in 2035 is simulated using the Community Multiscale Air Quality Modeling System (CMAQ) for California at 4 km x 4 km resolution. To assess climate impacts, meteorological conditions are generated for a baseline case and for a climate change case representative of the future Community Earth System Model (CESM1) simulation under the Representative Concentration Pathway (RCP8.5) scenario. The Model of Emissions of Gases and Aerosols from Nature (MEGAN) model is used to generate biogenic emissions using both baseline and climate-impacted meteorology. Emission control strategies were developed using the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System. SMOKE is used to grow and resolve anthropogenic emissions to 2035 based on expected emission control strategies from the California Air Resources Board. In addition, results from an electrical grid dispatch model in combination with transportation system modeling are used to consider the potential impact of wide-spread adoption of renewable electricity in tandem with electric vehicle deployment. Furthermore, the impact of climate correlated building energy consumption and the resulting emission changes are considered. For the first time, this work quantifies the impact of major factors on future air quality (e.g., aerosol and ozone) in California. For example, climate change alone could lead to an averaged increase of over 20 ppb in summer ozone, with the most prominent impacts in north central California. The number of days in which concentrations exceed health-based ozone standards also increase with the inclusion of climate impacts. The impact of climate is also significant for the concentration of $PM_{2.5}$, with an average increase over 14 $\mu g/m^3$ along the northern coast line of California, along with an average increase around 5 $\mu g/m^3$ over the San Francisco Bay Area and the Central Valley of California during the summer period. On the contrary, the effect of climate change results in an overall decrease of $PM_{2.5}$ during the winter period, with a maximum of 20 $\mu g/m^3$ within the Central Valley of California. Further comparisons will be made between the baseline and the alternative technologies case to understand the relative scale of impact between emission reductions from technologies advancement relative to impacts from climate including impacts on meteorology, biogenic emission, and end-use energy consumption. Finally, a comprehensive scenario will be simulated to include all contributing factors to understand the interactions and potential offsets among different factors.

12MG.7

Ambient Air Quality in Dhaka Bangladesh over Two Decades: Impacts of Policy on Air Quality.

Bilkis Begum, PHILIP K. HOPKE, *Atomic Energy Centre, Dhaka*

Samples of fine and coarse fractions of airborne particulate matter (PM) have been collected using a 'Gent' stacked filter unit from a semi-residential area at Dhaka from December 1996 until the present. The site is located at the Atomic Energy Centre, Dhaka University Campus which is a relatively low traffic area. During this period, many policies have been implemented to clean the air of Dhaka. Among them, banning of leaded-gasoline and two-stroke engines were implemented and a policy regarding green technology for brick burning is in progress. To observe the effects of the policy implementations, analyses were performed on this long-term (December 1996 to September 2015) data set of PM_{10}, $PM_{2.5}$, black carbon (BC), and lead (Pb). Year-wise concentrations of PM_{10}, $PM_{2.5}$, BC, and Pb were computed. There are characteristic seasonal variations for the PM_{10} as well as for the PM2.5 particles with elevated concentrations during the winter. The reasons for the high peaks during the winter are not only caused by seasonal fluctuations of the emissions, but also by meteorological effects. The statistical analyses of fine PM data indicate that fine PM concentrations in winter are also influenced by transboundary air pollution. Significant lead concentrations were still observed throughout the early 2000s. Pb is still being used in an uncontrolled manner in paints and there are also fugitive emissions from battery and other industries. It is likely that the major peaks are emissions from small battery reclamation efforts where there are no controls on emissions. These large spikes largely disappeared by 2006. The lead concentrations over the past decade are lower but still exceed the United States NAAQS value of 0.150μg/m^3. It is, therefore, essential to continue the fight for lowering lead level in air through the removal of lead in paints and through the control of emission from suspected industries especially lead based battery industries by regulatory measures. It can be observed from long-term data that the air quality of Dhaka has been stable over the past decade even though economic activity and the number of sources like passenger cars and brick kilns are increasing.

Source apportionments have been conducted for the periods of 2001-2002, 2005-2006, 2007-2009, and 2009-2015. The mean contributions of motor vehicles to $PM_{2.5}$ were 7.16, 5.62, 13.1, 3.19 μg/m^3, and the contributions to BC were 2.50, 0.38, 1.33, and 0.15 μg/m^3, respectively, showing the influence of the shift from gasoline and diesel to CNG as the primary transport fuel. The 2001-2002 results showed that vehicles normally produced about 50% of $PM_{2.5}$ particulate mass. The most recent source apportionment data (2009-2015) show that the contribution of BC from motor vehicles has also decreased following CNG adoption. Brick kilns continue to be a major source of PM and BC with mean $PM_{2.5}$ contributions of 2.2, 11.1, 5.6, 14.1 μg/m^3 and BC contributions of 1.37, 4.14, 1.53, 3.93 μg/m^3, respectively for the four, time intervals. Thus, there have been positive results for the governmental policies, but significant further reductions will be required, particularly from brick production, to achieve concentrations that meet typical health protective air quality standards.

12MG.8

Insights into PM2.5 Chemical Composition and Sources in Beijing Using an Extractive Electrospray Ionisation Long-Time-Of-Flight Mass Spectrometer (EESI-LTOF). YANDONG TONG, Veronika Pospisilova, Lu Qi, Giulia Stefenelli, Varun Kumar, Urs Baltensperger, Junji Cao, Rujin Huang, Andre S.H. Prévôt, Jay G. Slowik, *Paul Scherrer Institute*

Air pollution in megacities is of increasing importance due to rapid economic growth and urbanisation. Severe air pollution affects many fast-growing megacities in developing countries every year, including Beijing. Serious haze events in Beijing are mostly characterised by fine particulate matter ($PM_{2.5}$), which can either be directly emitted (primary) or formed by reactions of emitted gaseous precursors (secondary). Organic aerosol (OA) is a major component of atmospheric fine particulate matter and is responsible for much of the uncertainty in $PM_{2.5}$ sources, climate impacts, and health effects. Sources of primary organic aerosols (POA) are reasonably well understood, whereas many challenges remain in identifying and quantifying secondary organic aerosol (SOA) sources, because atmospheric ageing yields secondary compounds with similar functional groups, regardless of source, and existing online measurement techniques destroy important chemical information by thermal decomposition and/or ionisation-induced fragmentation.

We present results from an intensive online campaign in Beijing from the beginning of October to mid-December using a novel extractive electrospray ionisation long-time-of-flight mass spectrometer (EESI-LTOF) and a long-time-of-flight aerosol mass spectrometer (L-TOF-AMS). The EESI-LTOF enables rapid, real-time measurement of OA with soft ionisation by extracting aerosol into primary electrospray droplets (100 ppm NaI in 50:50 water:acetonitrile), resulting in $[M]Na^+$ adducts without thermal decomposition or ionisation-induced fragmentation. Although the EESI-LTOF shows an advantageous combination of near-molecular chemical information and high time resolution without sacrificing a linear response to mass, quantitative analysis is not yet completely established. Therefore, these measurements are complemented with an Aerodyne L-TOF-AMS equipped with a $PM_{2.5}$ aerodynamic lens, as well as measurement of organic gas species, black carbon and total carbon.

The campaign lasted for ten weeks, covering late autumn, heating season and transition period in between. During the 10-week campaign, 14 episodes with 24h-mean concentration higher than 50 $\mu g/m^3$ and five episodes with 24h-mean concentration higher than 150 $\mu g/m^3$ were observed. Distinctive difference is found between late autumn and heating season in winter from both L-TOF-AMS and EESI-LTOF. During the event in heating season (from 30 Nov to 3 Dec), aerosol composition was composed of organics (55%), nitrate (25%) and sulphate (10%), whereas in late autumn during the event (from 3 to 7 Nov), nitrate was the major component (40%), followed by organics (33%) and ammonium (15%). The different composition indicates different sources and processes between two periods. EESI-LTOF spectra suggest that biomass burning activities were enhanced relative to coal burning in the late autumn non-heating compared to the winter heating period. L-TOF-AMS and EESI-LTOF mass spectra are further investigated using positive matrix factorisation (PMF) as implemented by the multilinear engine (ME-2) with Source Finder (SoFi) interface. These results provide a quantitative description of the major primary and secondary sources influencing OA, as well as the effects of the recent change in fuel from coal to natural gas implemented in northern China in 2017.

12RA.1

Evaluation of the Second IMPROVE Equation. ANTHONY PRENNI, Jenny Hand, William Malm, Scott Copeland, Bret Schichtel, *National Park Service*

The Interagency Monitoring of Protected Visual Environments (IMPROVE) network provides the primary method for visibility monitoring at Class I Areas throughout the United States. Monitoring is conducted by collecting $PM_{2.5}$ and PM_{10} samples every third day at over 150 sites nationwide, with $PM_{2.5}$ samples being analyzed for chemical composition. Using these data, light extinction is reconstructed using the second IMPROVE Equation. Reconstructed extinction values are then used to calculate haze levels and estimate visibility. In addition to calculated light extinction from IMPROVE, the National Park Service directly measures aspects of visibility through optical measurements at a subset of IMPROVE sites using Optec NGN-2 integrating nephelometers. The optical measurements serve as a quality assurance check for IMPROVE, in that measured scattering from the nephelometers and reconstructed scattering from the IMPROVE Equation should be equivalent. During its development, the second IMPROVE Equation was shown to accurately estimate light scattering for a broad array of aerosol compositions and loadings. However, periodically revisiting the IMPROVE Equation is needed, as some of the relationships have been empirically-derived and may change with changing atmospheric composition. In this presentation, we compare measured light scattering to reconstructed light scattering from the second IMPROVE Equation at 11 sites over a 15 year period. The data suggest that the relationship between measured and reconstructed light scattering has changed over time, corresponding to systematic changes in the chemical and physical properties of the aerosol. One important implication of this is that trends based on calculated light scattering from IMPROVE measurements generally overestimate decreasing trends in measured light scattering. We present possible reasons for the discrepancies, discuss their implications, and propose a potential approach for correcting the IMPROVE Equation.

12RA.2

Measured In-situ Mineral Due Absorption Spectra. CHRISTOPHER ZANGMEISTER, James Radney, *National Institute of Standards and Technology*

Depending upon the locality, mineral dust aerosols generated from wind-blown soils can represent a significant fraction of local aerosol mass loadings. These aerosols are also capable of significantly affecting local energy budgets and radiative forcings. However, little is known about the absorption spectra of these particles. Of the published findings most focus on mineral dusts from desert regions. Here, we will present laboratory absorption spectra of aerosolized soil samples from locations across the United Sates (CA, IA, MD and MN) with land uses encompassing agriculture, forest and gravel roadbed road surfaces. Spectra were collected using a photoacoustic spectrometer with both a supercontinuum laser with a tunable wavelength and bandwidth filter and a diode laser allowing spectra to be measured from $\lambda = 405$ nm to 840 nm. We find that the measured spectra can be broadly grouped as either red clay-like or brown/gray dirt-like and possessing Absorption Angstrom Exponents (*AAE*) of > 7 or ≈ 3.5, respectively. Mass absorption coefficients (*MAC*) of sub-micron particles were also directly measured at 405 nm using a tandem differential mobility analyzer-aerosol particle mass analyzer with a photoacoustic spectrometer and condensation particle counter. MAC values were all less than 0.5 m^2/g and exhibited a moderate correlation with *AAE*. FT-IR spectra of each mineral dust enabled identification of materials within the sample set and were correlated to aerosol absorption spectra.

12RA.3

Towards Properly Decoding Trends in Wet Deposition of Inorganic Ions Related to Emissions and Climate Drivers.

Xiaohong Yao, LEIMING ZHANG, *Environment and Climate Change Canada*

A new approach was developed to preprocess monitored wet deposition data of inorganic ions for generating their decadal trends. Differing from traditional approaches which directly apply annual or seasonal averaged data to trend analysis tools, the proposed new approach makes use of slopes of regression equations between a series of study years and a climatology (base) year in terms of monthly averaged data. This approach was applied to the wet deposition data of SO_4^{2-}, NO_3^- and NH_4^+ at Canadian rural sites where with more than two-decade data, and the extracted decadal trends were properly linked to major driving forces such as emission reduction and climate anomaly. The decreasing trends in SO_4^{2-} and NO_3^- wet deposition were clearly observed, accompanied by increasing trends in the equivalent ratios of $NH_4^+/(NO_3^-+SO_4^{2-})$ and NH_4^+/NO_3^-, as a result of sharp decreases in SO_2 and NO_x emissions in recent years in Canada and the US. Some inconsistencies among wet deposition, equivalent ratio and emission were also seen mostly before 2000, which were identified to be caused either by climate anomaly or errors in estimated emissions. Long-term variations in NH_4^+ wet deposition were complicated and could not be simply attributed to known dominant factors; thus we confirm no cause-effect relationship was identified between emission and wet deposition for NH_4^+. The new approach proposed in this study yields more robust results than the traditional ones and stimulates towards properly decoding the trends in wet deposition.

12RA.4

Aerosol Liquid Water Driven by Anthropogenic Inorganic Salts: Implying Its Key Role in the Haze Formation over North China Plain. ZHIJUN WU, Yu Wang, Keding Lu, Song Guo, Limin Zeng, Yuanhang Zhang, Min Hu, *Peking University, China*

The aerosol liquid water content (ALWC) exhibits a profound impact on both air quality degradation and climate change. In this study, the ALWC was calculated based on (1) a thermodynamic model using long-term filter-based chemical composition data and (2) measured high-temporal-resolution size-resolved hygroscopic growth factors. The ALWC increased from 2% to 74% accompanying with the secondary inorganic faction in dry $PM_{2.5}$ rose from 24% to 55% and ambient relative humidity (RH) increased from 15% to 83% in the atmosphere over Beijing. During haze episodes, simultaneously elevated ambient RH levels and anthropogenic secondary inorganic mass concentrations resulted in an abundant ALWC. The condensed water could act as an efficient medium for multiphase reactions, thereby facilitating the transformation of reactive gaseous pollutants into particles and accelerating the formation of heavy haze. In particular, a greater ALWC is observed during the nighttime relative to the daytime. Unexpectedly, the secondary inorganic fraction in $PM_{2.5}$ increased with an increase in the ambient RH, which is a meteorological parameter independent of anthropogenic activities, indicating the presence of a feedback mechanism driven by Henry's law and thermodynamic equilibrium. As a particle uptakes anthropogenic compounds such as SO_2 and N_2O_5, its inorganic mass increases, thereby driving an increase in the water uptake. Then, a greater ALWC reduces the aerosol aqueous solution concentration, allowing for a greater uptake of inorganic compounds and completing the feedback mechanism. The ALWC was well correlated with the mass concentrations of both nitrate and sulfate, indicating that both nitrate and sulfate salts play key roles in determining the ALWC. Coincident with a significant reduction in SO_2 emissions throughout China, nitrates will become a dominant anthropogenic inorganic salt driving the ALWC. Thus, the abundance of the ALWC and its effects on the aerosol chemistry and climate should be reconsidered.

12RA.5

Coarse Aerosol Mass at Remote Sites across the United States. JENNY HAND, Bret Schichtel, Thomas Gill, *Colorado State University*

Understanding the spatial and temporal variability in coarse aerosol mass (CM = PM10 – PM2.5, mass of particles with diameters between 2.5 and 10 µm) is important for accurately characterizing and perhaps mitigating its environmental and climate impacts, which include influences on air quality, visibility, radiative forcing, hydrology, heterogeneous chemistry, biogeochemistry, and ecology. The spatial and seasonal variability of ambient CM was characterized at over 160 rural and remote sites in the United States in the Interagency Monitoring of Protected Visual Environments (IMPROVE) network. Monthly, seasonal, and annual means were computed for 2012 through 2016 to investigate the spatial and seasonal variability of CM. Regions with significant CM contributions to PM10 mass included the southwestern United States and southern Great Plains during the spring season and the central United States in spring, summer, and fall. The highest seasonal CM variability occurred in the West, peaking in spring months at sites in the Southwest near local and regional dust sources and in summer and early fall at sites in the Northwest, likely associated with local agricultural activity or biomass burning impacts. Eastern sites experienced relatively low CM seasonal variability. Trend analyses (2000–2016) indicated that CM and its contribution to PM10 have increased during specific seasons and across regions of the United States. Mitigating the environmental and climate impacts of CM will require improving source identification and characterization of its physico-chemical and optical properties.

12RA.6

Heterogeneity in the Concentration Distribution of Semi-Volatile Organic Compounds in the Surface Boundary Layer over the Tropical Forest in Central Amazonia. JIANHUAI YE, Patrícia C. Guimarães, Carla E. Batista, Igor O. Ribeiro, Adan Medeiros, Matthew Stewart, Yaowei Li, Matheus A. Tomoto, Daniel Wang, Dasa Gu, Rafael L. Oliveira, Sérgio Duvoisin Junior, Karena McKinney, Alex Guenther, Rodrigo A. F. de Souza, Scot T. Martin, *Harvard University*

Biogenic volatile organic compounds (BVOCs) significantly contribute to atmospheric oxidation capacity, and act as crucial parts in the carbon cycle of the atmosphere. Amazonia, the world's largest rainforest ecosystem, is one of the major sources of global BVOC emissions. Current atmospheric chemistry models have failed to accurately simulate BVOC oxidations over heterogeneous land surfaces, such as Amazon rainforest. Discrepancy has been observed in field studies between modeled and measured concentrations of BVOCs, as well as corresponding oxidants (e.g., hydroxyl radical). One of the reasons leading to this discrepancy is the non-uniform distribution of atmospheric BVOC species and their oxidants, owing to inefficient turbulent mixing and variable emissions (i.e., BVOC types and concentrations) over different forest sub-types. Semi-volatile organic compounds (SVOCs) formed from oxidation of BVOCs, are key precursors to the production of atmospheric particulate matter which plays a pivotal role in global climate change. Uneven BVOC distribution can lead to segregation of SVOC formations, resulting in segregated PM production in the atmospheric boundary layer over Amazonia. In this study, the hypothesis of SVOC heterogeneity is examined. The temporal and spatial distribution profiles of SVOCs from isoprene and monoterpene oxidation in Amazonia are investigated. Air samples are collected using unmanned aerial vehicle (UAV) technique, an emerging frontier in atmospheric chemistry. SVOCs are sampled by a custom-built sampler equipped with sorbent cartridges on the UAV, followed by chemical analysis using thermal desorption gas chromatography-mass spectrometry (TD-GC/MS) coupled with an online derivatization module. The SVOC data set obtained from this study, linking the diversity among VOCs and atmospheric PM production, will be used to better constrain current atmospheric chemistry models and provide insights on regional and global chemical transport in Amazonia.

12RA.7

Seasonal Changes in Organic Aerosol Composition in Ulaanbaatar, Mongolia. SKYLER SIMON, Audrey Dang, Brent Williams, Jay R. Turner, *Washington University in St. Louis*

Ulaanbaatar (UB), Mongolia is the coldest capitol city in the world and has faced persistent air quality challenges driven largely by wintertime space heating demands. For example, in 2016 the $PM_{2.5}$ mass concentration measured at the US Diplomatic Post in UB had an annual average >70 µg/m^3 with a wintertime (November-February) average >160 µg/m^3 and summertime (June-September) average <20 µg/m^3. Previous measurements demonstrate wintertime $PM_{2.5}$ is dominated by organic matter, perhaps as much as 85% of $PM_{2.5}$ mass. This is consistent with the primary sources of space heating being coal combustion in residential heating stoves in gers (yurts) and ger-area houses, heat-only boilers for schools and other small facilities, and combined heat and power plants that serve the central business district. However, there is little information on detailed organic speciation which could be valuable to understand emissions sources and health impacts.

We present results from organic speciation of 24-hour integrated ambient particulate matter samples collected on quartz filters at four sites across UB from January to April of 2013 [1]. These samples were thermally desorbed and analyzed off-line by gas chromatography – mass spectrometry using a Filter Thermal Desorption Aerosol Gas Chromatograph-Mass Spectrometer (Filter TAG). Individual molecular markers are identified and quantified, including polycyclic aromatic hydrocarbons which are known to have adverse health effects. Additionally, positive matrix factorization (PMF) solutions of binned chromatograms are used to investigate how seasonal trends in sources such as coal burning contribute to changes in ambient organic aerosol speciation [2].

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12RA.8

Fine Particulate Mass Scattering Efficiency and Refractive Index in the Central Amazonian Basin (ATTO station).

SAMARA CARBONE, Guilherme Santa Cecília, Luciana Rizzo, Joel Brito, Nga Lee Ng, Lu Xu, Jorge Saturno, Bruna A. Holanda, Florian Ditas, Christopher Pöhlker, Meinrat O. Andreae, Paulo Artaxo, *Federal University of Uberlândia*

To estimate the mass scattering efficiency (MSE) of PM1 and its individual components, linear regression models were applied to the aerosol scattering coefficient (measured by the Nephelometer, 525 nm) and to the PM1 main components (measured by the Aerosol Chemical Speciation Monitor, ACSM). In this study, the scattering coefficient and the PM1 variables represent the dependent and independent variables, respectively. During the dry season (August–December, 2014), in the central Amazonian basin, the average MSE obtained was 4.9 m2 g-1. In this season, the fine PM1 is dominated by chemical compounds from local and regional forest fires. Two specific episodes interfered in the analysis, and therefore were removed and analyzed separately. One of the episodes consisted of a volcanic eruption plume from Africa. The MSE during this episode was 8.9 m2 g-1, suggesting that the fine particles from this source were two times more efficient in scattering the solar radiation at 525 nm. During the wet season (February–May, 2015) the obtained average for MSE was 5.8 m2 g-1, slightly larger than the dry season. The larger value in this season could be due to the presence of chloride in the fine particles. In this time of the year, when the air pollution loading is low, it is possible to observe NaCl-riched particles, likely from the Atlantic Ocean. To study the MSE contribution of individual PM1 components a multi linear regression model (MLR) was used. Different grouping possibilities of the main components (except for BCe) were tested. Although this type of analysis can be biased by the number of chosen variables and presence of collinearity, all the possible groupings presented a similar trend for each season. That is, during the wet season the MSE values were lower for organics (1.2–3.2 m2 g-1), and larger for sulfate (or ammonium sulfate, 12.2–20.7 m2 g-1), while at the dry season the MSE for organics were larger (4.1–5.4 m2 g-1) and lower for sulfate (or ammonium sulfate, 3.2–4.8 m2 g-1). Wider variability of MSE is observed during the wet season, which could be related to the predominance of externally mixed particles and/or presence of more heterogeneous sources during this season.

Moreover, the Mie scattering code was used to estimate the refractive index by means of a closure study using the particle size distribution measured with the Scanning Mobility Particle Sizer (SMPS, TSI, mobility diameter=10-370 nm) and MLR model grouping results. The effective refractive index obtained for the dry season was 1.58-0.019i, and 1.61-0.0008i for organics. The real part of organic refractive index ranged from 1.4 to 1.77 and presented a rather stable and independent behavior as a function O:C, suggesting that at the central Amazonian basin, the PM1 refractive index for organics is not driven by oxidation.

12SA.1

High Resolution Analysis of Vehicle-related Organic Aerosols Observed at a Roadside Site in Hong Kong with the Application of TAG-ToF-MS. HAI GUO, Xiaopu Lyu, Wen Xu, John Jayne, Nathan Kreisberg, Allen H. Goldstein, Susanne Hering, Chak K. Chan, Xiangdong Li, Kin-Fai Ho, Douglas Worsnop, *Hong Kong Polytechnic University*

This is the first study on the real-time measurements of vehicle-related organic aerosols at a roadside site in Hong Kong with the aid of a Thermal-desorption Aerosol Gas Chromatography – Time of Flight – Mass Spectrometer (TAG-GC-ToF-MS). High-resolution measurements of hourly C_{13}-C_{40} n-alkanes and PAH species in particle- and gas-phase were carried out in winter 2017 near the Cross-Harbor Tunnel in Hong Kong. The results indicated that n-alkanes dominated over PAHs in $PM_{2.5}$, with the average concentrations of 87.3±4.6 and 5.9±0.3 ng/m^3 on weekdays, and 70.1±5.6 and 4.9±0.6 ng/m^3 on weekends, respectively. While PAHs showed typical bimodal pattern in daily cycle, n-alkanes only peaked at noon. Insight into the diurnal patterns of individual n-alkanes found that the large molecular (C_{21}-C_{33}) n-alkanes had both the morning and evening peaks, in contrast to the single peak of C_{13}-C_{20} n-alkanes at noon. Both CPI and Wax index implied that n-alkanes were almost exclusively derived from vehicle exhausts, except for one case when wax accounted for >20% of n-alkanes and many water-soluble substances (e.g. lauric acid, tetraethylene glycol and triethylene glycol) were detected with high abundances. PMF source apportionment analysis resolved two factors with one characterized by fluoranthene, pyrene, NO and NO_2, and the other one containing more chrysene, benzo[a]pyrene and CO. The results revealed that gasoline exhaust was the source of larger molecular n-alkanes (>C_{21}) and PAHs, and made higher contribution (13.9±1.3 µg/m^3) to the total organics in $PM_{1.0}$ than diesel exhaust (6.0±0.4 µg/m^3) which was responsible for the emissions of C_{13}-C_{20} n-alkanes. In the afternoon of a Sunday, the $PM_{1.0}$-bound total organics were even elevated by ~55 µg/m^3 by gasoline exhaust. The findings advance our understandings on emission characteristics of POA and formation mechanisms of SOA.

Keyword: TAG-GC-ToF-MS; n-Alkanes; PAHs; SOA; Roadside

12SA.2

A European-wide Intercomparison for Source Apportionment with Receptor and Chemical Transport Models.

CLAUDIO BELIS, Denise Pernigotti, Guido Pirovano, FAIRMODE WG3 Community, *European Commission - Joint Research Centre*

Assessing the performance of Source Apportionment (SA) model results is a key part of guaranteeing the quality of information on source contributions to be used in the development of pollution abatement strategies.

The performance of the source apportionment model applications was evaluated by FAIRMODE WG3, by comparing the model results for PM_{10} provided by 44 participants using a methodology based on performance indicators: z-scores and $RMSE_u$, with pre-established acceptability criteria (Belis et al., 2015).

Comparing models based on completely different and independent input data, such as receptor models (RMs) and chemical transport models (CTMs), provided a unique opportunity to cross-validate them. In addition, comparing the modelled source chemical profiles, with those measured directly at the source (e.g. SPECIEUROPE, Pernigotti et al., 2016) contributed to corroborate the chemical profile of the tested model results.

One of the distinctive features of this CTMs-RMs inter-comparison is that both kinds of models were applied on the same study area so called “reference site” thereby generating an unprecedented dataset of both source oriented and receptor oriented of source contribution estimates (SCEs). Moreover, the intercomparison was also an opportunity to compare the “tagged species” and “brute force” CTM SA approaches. The former keeps track of the emission source from which every chemical component derives while the latter is based on scenario analysis.

The most used RM was EPA- PMF5. RMs showed very good performance for the overall dataset (91% of z-scores accepted) and more difficulties were observed with SCE time series (72% of $RMSE_u$ accepted). Industry was the most problematic source for RMs due to the high variability among participants.

The results obtained with CTMs were quite comparable to their ensemble reference using all models for the overall average (>92% of successful z-scores) while the comparability of the time series was more problematic (between 58% and 77% of the candidates’ RMSEu were accepted). In the CTM models a gap was observed between the sum of source contributions and the gravimetric PM_{10} mass likely due to PM underestimation in the base case. Interestingly, when CTM results based only on tagged species methods were used in the reference, the differences between the two CTM approaches (brute force and tagged species) were evident. In this case the percentage of candidates passing the z-score and $RMSE_u$ tests were only 50% and 86%, respectively.

CTMs showed good comparability with RMs for the overall dataset (83% of the z-scores accepted), more differences were observed when dealing with the time series of the single source categories. In this case the share of successful $RMSE_u$ fell in the range 25% - 34%.

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12SA.3

A Global Scale Source Apportionment Scheme for Particulate Matter using the GEOS-Chem Global Atmospheric Chemistry Model. CARMEN LAMANCUSA, Kristina Wagstrom, *University of Connecticut*

As our society continues to develop and grow, it is necessary to expand our understanding of the impacts of atmospheric pollutant emissions on global scales. Researchers and regulatory agencies alike have used source apportionment as a powerful tool for quantifying and estimating these impacts on the regional scale. Towards expanding these capabilities from regional to global models, we have developed a new source apportionment scheme for the GEOS-Chem global atmospheric chemical transport model. The Global Particulate Matter Source Apportionment Technology (GPSAT) module represents the first incorporation into a global model. We have developed GPSAT within GEOS-Chem so that it will be available to all users in future versions of GEOS-Chem.

GPSAT can estimate contributions from different source classes (including locations and source types) without multiple model iterations or the need to create customized tracers. GPSAT is both computationally efficient and flexible. GPSAT allows us to develop a more complete picture of the impacts of intercontinental transport on global air pollutant concentrations. We will share estimates of the contributions from nine large, continent-scale, regions. We will also share further spatially refined estimates of contributions for the regions with the highest contributions globally. Finally we quantify the contributions of the 20 largest megacities to global air pollution concentrations using the average transport distance. We will specifically discuss the regions of the globe that most disproportionately impact global pollutant concentrations.

Through this project we have demonstrated an enhanced research tool (GEOS-chem with GPSAT) that will allow researchers throughout the globe to address a variety of scientific questions related to our understanding of long-range transport and the climate forcing contributions of different processes throughout the atmospheric component of the Earth System. Our goal in the analysis described here using GPSAT is to demonstrate the power and flexibility of the tool and thereby increase adoption by other researchers. The results from the analysis also provide necessary estimates for international discussions around air pollution. In addition, this analysis identifies areas most in need of focused attention in model improvement to potentially decrease model uncertainties. Finally, we provide a base-framework that other researchers can extend in the future to address the contributions from different processes throughout the entire Earth System and to identifying relative contributions to aerosol-climate feedbacks.

12SA.4

Excitation Emission Matrix Fluorescence Spectroscopy for Aerosol Source Identification. JAY RUTHERFORD, Neal Dawson-Elli, Igor Novosselov, Edmund Seto, Jonathan Posner, *University of Washington*

The inhalation of particulate matter (PM) is a significant health risk that can reduce life expectancy due to increased cardio-pulmonary disease as well as exacerbate respiratory diseases such as asthma and pneumonia. PM originates from natural sources, as well as anthropogenic sources such as combustion engines, cigarettes, and agricultural fires. The standard method for quantifying personal exposure to PM is measuring the mass concentration of $PM_{2.5}$ in air. Identifying the source of PM exposure can inform effective mitigation strategies and policies, but this is difficult to do using current personal monitoring techniques. Here we present a method for identifying PM source using excitation emission matrix (EEM) fluorescence spectroscopy and machine learning algorithms. We collected combustion generated $PM_{2.5}$ from wood smoke, diesel soot, and cigarette smoke using personal exposure monitoring filters. Following gravimetric analysis to determine mass concentration, the filters were extracted into cyclohexane for analysis by EEM fluorescence spectroscopy. The spectra obtained from pure sources were used as training data for identification of the same sources in mixed samples using machine learning. The method can identify source signatures with a 4 hour sampling time at a mass concentration of 5 $\mu g/m^3$. A pilot study of this EEM based source identification method is being evaluated as part of the Home Air In Agriculture - Pediatric Intervention Trial (HAPI) study in the Yakima valley of Washington using personal exposure monitoring units.

12SA.5

Fingerprinting Pre-monsoon Fine Aerosol Sources over Central Indo-Gangetic Plain. MANISH KUMAR, V.K. Sarma, R.S. Singh, Tirthankar Banerjee, *Banaras Hindu University*

Indo-Gangetic Plain (IGP) frequently experiences moderate to severe absorbing aerosols (smoke and dust) especially during pre-monsoon season (March-May), originating mostly from north western arid region. Atmospheric chemistry and potential sources of finer aerosols (PM2.5) were therefore, investigated at an urban location at central IGP during pre-monsoon for three consecutive years (2014-2016). Satellite derived aerosol optical properties i.e. aerosol optical depth (AOD), fine mode fraction (FMF), aerosol vertical profile and Aerosol Index (AI) were studied in synergy with ground observations, to evaluate the role of fine aerosols on columnar aerosol properties. The pre-monsoon aerosol characteristics revealed a substantial fraction of fine aerosols with average PM2.5 concentration of 75 µgm-3 varying from 12-195 µgm-3. The highest concentrations of finer aerosols contributed to 6-80% of the PM10. Terra-MODIS DB AOD (0.142-1.309) depict a sharp variability in the influx of both coarse and fine aerosols to the central IGP. Particle size in terms of Angstrom Exponent observed as high as >1.5, indicating co-existence of significant amount of finer aerosols. Further, a clear indication of trans-boundary movement of dust particle was noted using OMI-AI, with variation of aerosol extinction coefficients. Chemical signatures in association with air mass back trajectory further identified the potential sources of aerosols, distributed over north-western arid regions, with mixing of locally emitted finer aerosols. Finally, the source apportionment of pre-monsoon finer aerosol through multivariate and hybrid receptor models highlighted some key sources of aerosol over the region.

12SA.6

Real Time Source Quantification of Secondary Organic Aerosol in Zurich Using Extractive Electrospray Ionization Time-Of-Flight Mass Spectrometry (EESI-TOF). LU QI, Giulia Stefenelli, Veronika Pospisilova, Yandong Tong, Christoph Hueglin, Martin Rigler, Xinlei Ge, Mindong Chen, Urs Baltensperger, Andre S.H. Prévôt, Jay G. Slowik, *Paul Scherrer Institute*

Real-time, in situ molecular composition measurements of the organic fraction of fine particulate matter (PM2.5) remains challenging, hindering a full understanding of the climate impacts and health effects of PM2.5. Unlike primary organic aerosol (POA), which has been studied extensively and relatively well characterized, the source contributions and mechanistic studies of secondary organic aerosol (SOA), which typically dominates OA, remains unclear due in large part to the limitations of existing measurement systems. In this study, a new extractive electrospray ionization time-Of-flight mass spectrometer (EESI-TOF), which OA composition on a near-molecular level without fragmentation or thermal decomposition, was deployed to measure OA in downtown Zurich, Switzerland, during winter 2017. Positive matrix factorization (PMF) and the Multilinear Engine (ME-2) were applied to separate the detected SOA species into several factors, relating these factors to POA and SOA sources. Moreover, some of the factors agreed well with factors retrieved from PMF analysis of the mass spectra of a co-located Aerodyne AMS.

Eleven factors were selected to explain the EESI-TOF data, including six SOA factors (two aged emissions, one aged pollution event, two photo chemistry factors, one nitrogen containing factor), four POA factors (cooking, two special events, one local wooding burning emission) and one factor dominated by nicotine. The two local aged emission factors had a negative correlation with temperature, the temporal variation of one factor is distinct at low temperature and another one factor varied at high temperature. The factor enhanced at lower temperatures contains compounds with lower carbon and oxygen numbers, and correlates with phthalic acid (C8H6O4) and glutaconic acid (C5H6O4). The photo-chemistry factors are similar to laboratory spectra generated from oxidation of -pinene by ozone and hydroxyl radicals. The local wooding burning emission factor was related to domestic wood burning for heat and peaks from 18:00 to 6:00 o'clock, correlating with levoglucosan (C6H10O5) and the hydroperoxide (C8H12O6). Also, nitrocatechol (C7H7NO4), suggested to be another tracer of secondary biomass burning, exhibited a similar diurnal pattern as local wood burning emission factor with a nocturnal peak. The nicotine factor correlates well with a cigarette smoke factor retrieved from the AMS PMF, as well the C5H10N+ ion identified as a cigarette smoke tracer. These findings improve our understanding of SOA sources and production, highlighting in particular the complexities of biomass burning evolution in the atmosphere.

12SA.7

Impact of a Shrinking Saline Lake (Salton Sea) on Regional Dust Deposition and Composition. ALEXANDER FRIE, Alexis Garrison, Mia Maltz, Jon Botthoff, Steve Bates, Timothy Lyons, Emma Aronson, Roya Bahreini, *University of California Riverside*

Shrinking saline lakes and the formation of large emissive lake beds (playas) are increasingly common as demand for water resources in arid regions grow. The Salton Sea (SS) is a saline lake with water levels receding, exposing the playa underneath. The resulting playa exposures are raising air quality concerns in the SS air basin. SS Playa dust emissions are compositionally distinct from other regional particulate matter (PM) sources and typical mineral dust, allowing for tracing of playa emissions. Previous work has identified SS playa influences on ambient PM_{10} on short time scales, attributing ~10% of PM_{10} mass and >40% of PM_{10} Na to playa sources.[1] To quantify the impact of SS playa emissions on PM mass and composition on longer timescales and with greater spatial resolution, monthly depositional samples are collected from five sites in the SS Basin and Coachella Valley from May 2017-2018. The total elemental and soluble anion concentrations within these samples are respectively measured with inductively-coupled plasma mass spectrometry (ICP-MS) and ion chromatography. These data will be input into Positive Matrix Factorization (PMF) software to isolate source contributions and determine source profiles of the deposited dust. Additionally, enrichment factors are calculated and used to explore compositional differences in depositing dust at each site, including those driven by playa exposures. Preliminary results show samples from sites closest to the SS playa surfaces have high enrichments of sulfate, Na, Ca, and Se, indicating compositional changes driven by playa emissions. These data provide insight into the regional importance of SS playa emissions and their effect on PM composition.

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12SA.8

Positive Matrix Factorization of SEM Based Individual Particle Results from the Middle East: A Comparison of Data Sets from Kuwait Collected during Two Time Periods. Johann Engelbrecht, GARY CASUCCIO, Traci Lersch, *RJ Lee Group, Inc.*

Aerosol sampling and analyses programs mandated by U.S. military and government agencies provided detailed characterization of ambient particulate matter in the Middle East airshed. The U.S. Army Environmental Hygiene Agency, re-designated as the U.S. Army Center for Health Promotion and Preventive Medicine (USACHPPM), designed an investigation to produce data to be used to assess the health risk of oil well fires to U.S. troops involved in Operation Desert Storm. Sampling began in Kuwait and Saudi Arabia in early May 1991 and continued through Dec 1991. The goal was to determine the magnitude and extent of pollutants released to the atmosphere from the burning of oil wells. Fifteen years later, a study to generate information on the chemical and physical properties of aerosols collected at military deployment locations in the Middle East was initiated by the U.S. Department of Defense. The purpose was to characterize the aerosols and to provide information that could be used to assess human health effects from exposure to ambient particulate matter at Middle Eastern military bases. Aerosol and bulk dust samples were collected for evaluation over a period of approximately one year following 2005 at fifteen military sites.

For both studies, ambient particulate matter was analyzed by scanning electron microscopy (SEM). An SEM equipped with an energy dispersive X-ray spectroscopy (EDS) system was used to obtain information on the chemical and morphological composition of individual particles. This furthermore provided insight on mineralogical relationships, source identification, and other particle features such as surface coatings. Automated scanning electron microscopy (SEM) techniques were employed to measure particle size, morphology, and composition for a large number of individual particles to produce quantitative data at each location.

The automated SEM/EDS data from the Middle East ambient samples are being used to develop source factors applying positive matrix factorization (PMF). The derived mineralogical composition of the individual particles is also a signature of the region’s geology. Examples include the high quartz content of the four Kuwait sites, the high percentage of calcite in the United Arab Emirates samples, the high dolomite content of the Al Asad samples, and the titaniferous magnetite dust from Djibouti. Further, the automated SEM results also provided direct measurements on carbon chain agglomerated structures, tracers of the oil fire plumes. This investigation examines the source factors established from PMF; evaluates the impact of these emissions on the Middle East ambient environment; and compares the results obtained from multiple locations in the region over two different time periods.

13AC.1

Biogenic New Particle Formation: From Pristine to Polluted Environments. LUBNA DADA, Martin Heinritzi, Mario Simon, Chao Yan, Dominik Stolzenburg, Katrianne Lehtipalo, Markku Kulmala, Jasper Kirkby, CLOUD Collaboration, *University of Helsinki*

Atmospheric aerosols affect Earth’s radiative energy balance. New particle formation (NPF) by gas-to-particle conversion is estimated to contribute to more than half of global cloud condensation nuclei. Previously, it was thought that NPF can only occur in the presence of sulfuric acid vapour and that ions play only a minor role in the process. However, the CLOUD (Cosmics Leaving OUtdoor Droplets) experiment at CERN has shown that pure biogenic particles can form from organic precursors in the absence of any other vapor, including sulfuric acid (Kirkby et al., Nature 533, 2016), and, moreover, that ions are important to stabilise the embryonic particles. Formation of pure organic particles has also been observed in the real atmosphere, making the phenomenon important for further investigation (Bianchi et al., Science 352, 2016).

Here we present results from CLOUD experiments on pure biogenic NPF and early growth under realistic atmospheric conditions. Our aim is to understand the interactions between the environment and different precursor volatile organic vapours by introducing an individual monoterpene, a sesquiterpene and isoprene, and then combining them to form what we call a biogenic “soup”. Using different concentrations of the biogenic soup at temperatures of -25, 5, 25 ^{o}C, we measured the formation and growth rates of pure biogenic particles. We investigated the influence of NOx on the production of the highly oxygenated biogenic molecules (HOMs) responsible for NPF and growth. We also studied the effect of various ionisation rates from zero to natural cosmic rays to the CERN pion beam to demonstrate the different layers of the atmosphere. Finally, in order to understand the boundary between pristine and polluted environments, we added sulfur dioxide and ammonia to the chamber and measured where the transition occurs between pure biogenic- and sulfuric acid-driven nucleation.

Our measurements of pure biogenic nucleation under realistic environmental conditions will help to understand nocturnal NPF in the absence of sulfuric acid, and also of NPF in pristine environments such as during the pre-industrial period or in the Amazon at low and high altitudes.

13AC.2

The Birth of Haze: Molecular Understanding of New Particle Formation in Beijing. YING ZHOU, Chao Yan, Juha Kangasluoma, Yonghong Wang, Federico Bianchi, Tommy Chan, Biwu Chu, Lubna Dada, Kaspar Rudolf Dällenbach, Yueyun Fu, Xucheng He, Liine Heikkinen, Yiliang Liu, Yiqun Lu, Qingxin Ma, Pekka Rantala, Gan Yang, Rujin Yin, Joni Kujansuu, Tuukka Petäjä, Yongchun Liu, Lin Wang, Jingkun Jiang, Markku Kulmala, *Beijing University of Chemical Technology*

New Particle Formation (NPF) is an important source of atmospheric aerosol particles in the atmosphere that have known impacts on health, visibility and climate. Additionally, recent studies discuss the potential role of newly born particles in haze formation. In the last decade, NPF has been investigated both in ambient environments, such as in boreal forest or mountain slopes as well as in atmospheric simulation chambers, especially in the CLOUD experiment at CERN. Despite the large number of studies, only few NPF observations from highly polluted urban environments have been reported and the detailed understanding of such cases is still insufficient.

In order to better understand the complexity of air pollution, and especially the formation of haze events in Chinese megacities, we are conducting comprehensive long-term measurements in downtown Beijing. The newly constructed measurement station is equipped with state-of-the-art instruments for aerosol research focusing on new particle formation. The physical properties of aerosol particles are measured with a Particle Sizer Magnifier (PSM), a Neutral cluster and Air Ion Spectrometer (NAIS) and a scanning mobility particle sizer with diethylene glycol as the working fluid (DEG-SMPS). The chemical characterization of aerosol particles as well as the nucleating clusters is performed with chemical ionization mass spectrometers (CIMS) using different types of chemical ionization techniques (such as NO_3^- and I^-), a regular atmospheric pressure interface time-of-flight mass spectrometer (APi-TOF) a filter inlet for gases and aerosols mounted in front of a CIMS (FIGAERO-CIMS) , and a time of flight aerosol chemical speciation monitor (TOF-ACSM).

During the measurement period in urban Beijing, we observed a frequent occurrence of NPF events. We classified these events into three groups according to the air pollution index: clean days, moderately polluted days, and highly polluted days, respectively. Formation rate, growth rate and condensation sink were calculated for each of the groups. Additionally, the behavior of gas phase sulfuric acid and highly oxygenated molecules were analyzed and compared among the different pollution categories.

Our study provided new and comprehensive insights into aerosol formation, growth and thereafter haze formation in a molecular level in urban Beijing that is needed for more efficient emission control strategies in the highly developing North China Plain.

13AC.3

Chemistry of New Particle Growth During Spring Time in the Seoul Metropolitan Area, Korea. HWAJIN KIM, Qi Zhang, *Korea Institue of Science and Technology*

New particle formation and growth events (NPEs) were frequently observed (24 out of 60 days) during April 14 to June 15, 2016 in the Seoul metropolitan area (SMA). In this study, we investigated the chemical mechanisms of new particle growth based on measurements conducted using an aerodyne high resolution time-of-flight aerosol mass spectrometer (HR-AMS) and a scanning mobility particle sizer (SMPS). Both instruments were deployed as part of the KORUS-AQ campaign (Korea-US Air Quality study). NPEs usually started in the afternoon between ~12:00 and 13:00 with the appearance of an ultrafine mode at < 20 nm (in mobility diameter, D_m, measured by a SMPS operating in the range 18-947 nm) followed by the growth of this modal diameter to ~45-80 nm during the next ~6-12 h. The growth rate was on average 4.48 ± 1.39 nm/h. Comparing to the non-NPE days, our results indicate that NPEs in SMA occurred when the concentration of preexisting particles was lower (15 vs 23 $\mu g/m^3$), higher ozone (48 vs 27 ppb), stronger solar radiation (2.13 vs1.04 MJ/m^2), and drier conditions (36 vs 65%). The evolution of the size-resolved chemical composition of new particles was investigated based on the HR-AMS size distribution measurements. The results showed that the concentration of LV-OOA (low volatile oxidized organic aerosol) and/or sulfate increased when NPEs occurred and that the concentrations of those species increased continuously as particles grew. Nitrate concentration also increased at the later stage of the particle growth. These results indicate that the frequently occurring NPEs in Seoul during spring were mainly driven by intensive formation of secondary species by photochemical reactions. Details on the mechanisms of NPEs in SMA will be discussed.

13AC.4

Molecular Understanding of the Suppression of Organic Nucleation by Isoprene. Martin Heinritzi, Lubna Dada, Mario Simon, Dominik Stolzenburg, Lukas Fischer, Andrea C. Wagner, ANDREAS KÜRTEN, Jasper Kirkby, Joachim Curtius, *Goethe University Frankfurt*

The formation of new particles in Earth's atmosphere out of gaseous precursors contributes around 50% to global aerosol loadings and has thus large climatic impacts. It was recently shown that the highly oxygenated products of monoterpene (C10H16) oxidation are able to contribute to nucleation and also nucleate on their own, without the help of other precursors, at atmospherically relevant concentrations (Kirkby et al., 2016). However, atmospheric observations show that even if there are sufficient monoterpenes available, new particle formation is suppressed when isoprene (C5H8) is also present at low ppb levels. These observations were made e.g. in the Amazon basin and in the Southeast of the United States, both of which experience high isoprene levels. It was proposed that OH depletion by isoprene inhibits nucleation (Kiendler-Scharr et al., 2009). However, field measurements have reported undiminished OH levels in the presence of isoprene, and it was shown that isoprene oxidation is capable of recycling OH. So it remains an open question as to why isoprene seems to inhibit biogenic nucleation under otherwise favorable conditions for the formation of new particles.
Here, we use data from the Cosmics Leaving OUtdoor Droplets (CLOUD) experiment at CERN, Geneva, to investigate this mechanism. The CLOUD experiment is a very clean and controlled aerosol reactor, equipped with a suite of state-of-the-art mass spectrometers and particle counting instruments that enables us to study nucleation under precisely controlled conditions. We measured the oxidation products of the monoterpene α-pinene in the presence and absence of isoprene, using a nitrate based Chemical-Ionization Atmospheric Pressure Interface Time-Of-Flight mass spectrometer (CI-API-TOF).

We find that nucleation of 1.7 nm particles in the α-pinene/ozone system is reduced when isoprene is present. We also find a reduction of the growth rate of particles in the small size range in the presence of isoprene. We are able to explain these observations at the molecular level due to changes in the composition of Highly Oxygenated Molecules (HOMs) that drive nucleation and growth.

We discuss our findings with respect to the results from Kiendler-Scharr et al., 2009. Our results can help explain the absence of nucleation in isoprene rich environments, such as the Amazon and the Southeast of the United States and may help to increase the accuracy of global aerosol models in the future.

13AC.5

Impact of SO2 on Particle Formation and Growth from α-Pinene Ozonolysis. CHRIS STANGL, Justin Krasnomowitz, Murray Johnston, Shanhu Lee, *University of Delaware*

Secondary organic aerosol (SOA) plays a major role in atmospheric nanoparticle growth, and greatly impacts climate by enhancing cloud condensation nuclei (CCN) number. Biogenic emissions, in particular isoprene and monoterpenes, represent the major volatile precursors to organic aerosol formation, accounting for roughly 90% of the global SOA flux. Although the potential for these species to form SOA has been studied extensively, less remains known about how interactions with anthropogenic emissions affects this process. In this work, the effects of SO_2 on nanoparticle formation and growth from α-pinene ozonolysis were studied in a flow tube reactor. Experiments were conducted in the presence of 60 nm monodisperse ammonium sulfate seed particles under a 4-minute residence time, and at atmospherically relevant levels of the gas-phase reactants. Under dry (RH < 10%) conditions, significant growth of the seed particles was observed from α-pinene ozonolysis, with very little new particle formation under the conditions used. Following the addition of SO_2, new particle formation was observed due to the oxidation of SO_2 to H_2SO_4 by OH radical and/or the stabilized Criegee Intermediate (sCI) formed during ozonolysis. Growth of the seed particles as well as the total amount of secondary aerosol produced, however, were found to be reduced in the presence of SO_2, likely due to consumption of OH by SO_2 that would otherwise oxidize additional α-pinene molecules, or reaction with sCI to inhibit the formation of highly oxidized molecules (HOMs) that could condense to the particle phase. Elemental composition analysis of the grown seed particles was conducted in the presence and absence of SO_2 using the Nano Aerosol Mass Spectrometer (NAMS), and revealed a larger sulfur-to-carbon mole fraction ratio of the particles exposed to SO_2, suggesting a significant sulfuric acid contribution to particle growth. Additional experiments were carried out with cyclohexane present in the flow tube to investigate the effect of OH removal on particle formation and growth. With cyclohexane, growth of the seed particles by α-pinene was decreased, indicating a significant OH contribution to HOM formation under the conditions examined. With both cyclohexane and SO_2 present, growth was decreased even further, however particle formation was still observed to a similar extent as without cyclohexane, suggesting that the sCI plays an important role in SO_2 oxidation. These results suggest that SO_2 is able to inhibit SOA production by reducing the amount of HOMs formed, and this effect may lead to a reduction in CCN number in locations where forested air can become infused with anthropogenic pollutants, such as the southeastern U.S. Ongoing work entails investigating the effect of SO_2 on particle formation and growth with other SOA precursors, seed particle compositions and higher relative humidities.

13AC.6

Mechanisms That Control the Contribution of Aromatic Highly Oxidized Multifunctional Compounds (Homs) to Initial Particle Growth in the Atmosphere. MINGYI WANG, Dexian Chen, Mao Xiao, Victoria Hofbauer, Penglin Ye, Alexander Lucas Vogel, Qing Ye, Roy Lee III Mauldin, Neil Donahue, *Center for Atmospheric Particle Studies, Carnegie Mellon Uni*

Organic condensation from the gas phase to the particle phase contributes to the initial growth of freshly nucleated particles and causes secondary organic aerosol (SOA) formation (Tröstl et al., 2016). SOA, in turn, may comprise well over half of the total fine-particle mass in the lower atmosphere, contributing to and possibly dominating health effects that include more than 4 million premature deaths per year (Apte et al., 2015). However, to what extent organic condensation affects the initial growth of newly formed particles smaller than 10 nm remains in doubt, and the mechanism forming "condensable" organic vapors is even less certain.

Ozonolysis of terpenes, followed by peroxy-radical auto-oxidation via a succession of internal H-atom transfer reactions, produces highly oxidized multifunctional compounds (HOMs) within a few seconds after the initial attack of ozone (Jokinen et al., 2014). This dominates new-particle formation in regions dominated by biogenic emissions. However, these processes can be suppressed substantially in the anthropogenic atmosphere, nitrogen oxides (NOx) can perturb peroxy-radical chemistry (Yan et al., in preparation). However, the urban atmosphere contains far more than NOx, laboratory studies have reported HOM formation from OH-triggered oxidation of aromatic hydrocarbons, highlighting the potential contribution of aromatic HOMs to nucleation and initial particle growth in the anthropogenic environment (Molteni et al., 2018).

In order to understand the role of aromatic hydrocarbons in new-particle formation, especially the initial growth of nucleated particles, experiments using toluene, 1,2,4-trimethylbenzene and naphthalene as oxidation precursors were conducted under typical urban conditions in the “Cosmics Leaving OUtdoor Droplets” (CLOUD) chamber. We measured the particle-phase volatility of aromatic HOMs via thermal desorption using an iodide-adduct Long Time-of-Flight Chemical-Ionization Mass Spectrometer equipped with a Filter Inlet for Gases and AEROsols (FIGAERO-LToF-CIMS). The particle-phase volatility measurements confirm that oxidation products of toluene, trimethylbenzene and naphthalene can and do contribute to the initial growth of newly formed particles. Naphthalene oxidation forms the least volatile products and thus is the strongest contributor to growth among the three aromatic precursors. Toluene-derived HOMs have slightly lower volatility than TMB-derived HOMs, and their volatility distribution is similar to that of monoterpene-derived HOMs. More detailed exploration of the oxidation mechanism suggests that rapid progression through multiple generations of oxidation is more pronounced in aromatic hydrocarbons, which resulting in more oxidation but crucially also favoring functional groups with much lower volatility per added oxygen atom. Ultimately, the relative contribution of the different aromatic precursors to nucleation and growth in highly polluted urban atmospheres will depend on the volatility distribution of the products as well as the relative concentrations of the precursors. It is likely that naphthalene will always dominate growth of the smallest particles, whereas the alkylbenzenes may overtake naphthalene once the particles have grown beyond the point where the Kelvin effect strongly influences the condensation driving force (roughly 10 nm diameter).

13AC.7

Thermodynamics of Neutral Ternary (H2SO4-H2O-NH3) New Particle Formation Derived from CLOUD Chamber Measurements. ANDREAS KÜRTEN, *Goethe University, Frankfurt*

Ammonia is an important atmospheric trace gas that is responsible for the formation of a large fraction of secondary aerosol. The largest source of ammonia is anthropogenic emissions. Recently, it was estimated that eliminating agricultural emissions of ammonia could reduce PM2.5 by up to 50% over large regions of Europe (Pozzer et al., 2017). Regarding the number concentration of aerosol particles and cloud condensation nuclei (CCN), ammonia is also important as it can efficiently enhance new particle formation (NPF) due to an acid-base stabilization mechanism together with sulfuric acid (Kirkby et al., 2011).

New particle formation rates from several hundred CLOUD chamber measurements were recently used to parameterize NPF rates as a function of sulfuric acid, ammonia, and ion concentration over a wide range of temperatures (~208 to 298 K) (Dunne et al., 2016). The implementation of this parameterization was used in the GLOMAP (Global Model of Aerosol Processes) model to estimate the contribution of individual nucleation channels (e.g., binary neutral, ternary neutral, etc.) to global aerosol and CCN formation. These simulations indicate that more than half of all particle formation in the troposphere involves ammonia. Kürten et al. (2016) also highlighted the strong enhancement of ammonia on NPF, even when ammonia was present at tiny mixing ratios (pptv-range). However, the reported parameterization by Dunne et al. (2016) does not give any insight into the thermodynamics (i.e., the evaporation rates) of the nucleating sulfuric acid-ammonia clusters. Evaporation rates reported in the literature are mainly based on quantum chemical calculations, with rare exceptions (e.g., Hanson et al., 2017).

Here we use the CLOUD NPF rates from Dunne et al. (2016) and Kürten et al. (2016) to derive the evaporation rates for the most important nucleating clusters. We use an acid-base scheme in the nucleation and growth model that was recently introduced by Kürten et al. (2018). The evaporation rates are determined by minimizing the average error between modeled and measured NPF rates. Applying this method over a wide range of experimental conditions (temperature, ammonia and sulfuric acid concentrations), the evaporation rates for the smallest sulfuric acid-ammonia clusters can be determined (up to the tetramer containing four sulfuric acid and four ammonia molecules).

The results of this study will be reported and the derived thermodynamic data will be compared to literature values. In addition, further model results will be discussed, e.g., the influence of the condensation sink on new particle formation and growth can be tested, as well as the influence of ammonia on the growth rates of particles.

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13AC.8

Free Tropospheric New Particle Formation Observation from High Altitude Sites around the Globe. FEDERICO BIANCHI, Claudia Mohr, Diego Aliaga, Qiaozhi Zha, Xuemeng Chen, Otso Peräkyla, Joonas Enroth, Yee Jun Tham, Liine Heikkinen, Fernando Velarde, Juha Kangasluoma, Angela Marinoni, Stefania Gilardoni, Mikael Ehn, Katrianne Lehtipalo, Paulo Artaxo, Mikko Sipilä, Marcos Andrade, Radek Krejci, Armin Hansel, Paolo Laj, Tuukka Petäjä, Neil Donahue, Douglas Worsnop, Markku Kulmala, *University of Helsinki*

Atmospheric aerosols affect the climate directly by interacting with the incoming solar radiation and also indirectly via acting as cloud condensation nuclei (CCN) and thus impacting the cloud albedo and lifetime. A significant fraction of atmospheric CCN arises from new particle formation (NPF) of which 35% are directly formed in the free troposphere. During the last decade, several nucleation studies have been published based on field observations. However most of the studies are conducted within the planetary boundary layer (PBL), and only little information is available of NPF in the free troposphere (FT). The aim of this presentation is to elucidate the chemical fingerprints of the species involved in the NPF in the upper troposphere.

In the last years, we have used a number of state-of-the-art instruments to retrieve chemical information about the vapours involved in NPF in the FT: First at the Swiss high alpine research station Jungfraujoch (3580 m asl), then at the Himalayan Nepal Climate Observatory Pyramid (NCO-P) site on the southern slope of the Himalayas (5079 m asl), not far from Everest base camp and currently (December 2017 – May 2018) at the Chacaltaya station (5300 m asl) located in Bolivia. Previous studies have already shown that in all of these locations NPF takes place frequently, albeit without chemically specifying the involved vapours.

We deployed the most advanced instrumentation for studying new particle formation in all of the three locations. The basic set of instruments consists of an atmospheric pressure interface time-of-flight mass spectrometer (APi-TOF), a particle size magnifier (PSM) and a neutral cluster and air ion spectrometer (NAIS). The APi-TOF measured the chemical composition of either the positive or negative gas phase ions and ion clusters throughout many NPF events, and when equipped with a chemical ionization source (CI-APi-TOF) it also provided information on the chemical composition of the neutral species. Additional important instrumentation added in the latest measurement at the Chacaltaya station are a CI-APi-TOF equipped with a FIGAERO (Filter Inlet for Gases and AEROsols), and two ACSMs (Aerosol Chemical Speciation Monitor) for chemical composition measurements of larger atmospheric particles; and a proton transfer reaction time-of-flight mass spectrometers (PTR3TOF) to gain information on volatile organic compounds and their oxidation products, which are important precursors of organic aerosol.

In this presentation, we will focus on the results collected during the latest measurement campaign at Chacaltaya station, Bolivia, and compare them against the findings from previous high-altitude measurement campaigns from Jungfraujoch and Himalaya. We will present a detailed analysis of the evolution of the newly formed particles during NPF as well as the chemical composition of the small clusters measured with the (CI-)APi-TOFs. Finally, we will highlight the importance of these processes in order to understand the aerosol conditions in the pre-industrial era where information is really scarce.

13AP.1

On the Inherent Measurement Uncertainty of Miniaturized PM Sensors. PAUL MAIERHOFER, Georg Röhrer, Alexander Bergmann, *Graz University of Technology*

Serious adverse health effects of PM on the human body raise a public desire for highly integrated, cost-effective and easy-to-use PM sensors. As the chase for smaller and smaller PM sensors is currently at an all-time high, it is not only fruitful but also necessary to have a closer look at limitations we encounter. Despite all the evident benefits miniaturized sensors are bringing, there is an inherent drawback in measurement accuracy, which is closely related to the discrete nature of particulates suspended in air. The miniaturization of those devices not only leads to smaller footprints of the devices themselves but also to smaller samples of air being measured. Even if a perfect measurement system is assumed which is able to correctly sense all particles in mass in any volume of air that is drawn through it, there is an inherent uncertainty in assigning a PM2.5 value representative for the ambient. This stems from the fact that particles are discrete and therefore stochastically distributed in the air. Consequently, there is an uncertainty according to counting statistics, as the number of investigated particles in small samples of air is also low. Additionally, the distribution of particle sizes and masses is not ideally captured by an arbitrarily small sample size especially since the size distribution of particles extends over orders of magnitudes. This distribution related uncertainty adds to the uncertainty resulting from counting statistics.

We investigated the expected measurement uncertainty for the described system by analytical means leading to the conclusion that both the exact size distribution of particles as well as the sample size have a major impact on the measurement uncertainty. By transformation of variables and use of the central limit theorem, this uncertainty was quantified and evaluated for various situations. Simulations using random numbers generated by a Monte Carlo algorithm were used to back the analytical results.

For an exemplary size distribution of urban aerosol at a concentration of PM2.5 = 25 $\mu g/m^3$ and a sample size of 1 ml the 1 σ standard deviation is around 37% resulting solely from the fact that the number of particles in the sample is small, disregarding all other potential measurement errors.

As a conclusion the miniaturization of PM sensors and the connected miniaturization of microfluidic devices and therefore the sample size, leads to a significant uncertainty of the measurements. The only way to avoid these uncertainties is to avoid small samples e.g. by taking longer measurement times or guaranteeing relatively high flow rates, which seems contrary to miniaturization. Said uncertainty is not negligible, but is to be taken into account when developing future sensors.

13AP.2

How Uncertainties in Measurements and Choice of Regression Method Affect Inference from Data. SANTTU MIKKONEN, Mikko Pitkänen, Tuomo Nieminen, Antti Lipponen, Antti Arola, Kari Lehtinen, *University of Eastern Finland*

When analysing dependencies of two or more measured variables, regression models are usually applied. Regression model can be linear or nonlinear, depending on the data. Standard regression models assume that the independent variables of the models have been measured without error and the models account only for errors in the dependent variables or responses. In cases where the measurements of the predictors contain error, the estimation with the standard methods, usually Ordinary Least Squares (OLS), do not tend to the true parameter values, not even asymptotically. In linear models, the coefficients are underestimated but in nonlinear models, the bias is likely to be more complicated.

Measurement errors in each variable of the model must be taken into account in the regression analysis by applying some errors-in-variables (EIV) regression. In this study, we compared OLS regression results to six different regression methods (Deming regression, Principal component analysis regression, orthogonal regression, Bayesian EIV regression and two different bivariate regression methods) known to be able to take account errors in variables and provide (at least asymptotically) unbiased estimates.

We simulated a dataset mimicking new particle formation rate (J_3) and sulphuric acid concentration (H_2SO_4) reported from CLOUD-chamber measurements in CERN. Both variables are known to have substantial measurement error and thus they are good test variables for our study. Additionally, the relationship of logarithms of these variables is quite often described with linear OLS regression and thus the inference may be flawed.

The data were simulated using model $\log10(J_3)=\beta*\log10(H_2SO_4)+\alpha$ with the “true slope” β=3.3 and with measurement error comparable to bias in true measurements. OLS regression gave slope of 1.7 and the EIV models gave slopes in range 2.48-4.05, depending on the procedure, how they account for the measurement error. The biases and sensitivity of different regression methods were compared with simulations with different error rates and different sample sizes. All methods had high uncertainty with samples smaller than 10 observations but with larger samples, all methods converged rapidly to their peculiar level. When the variance of H_2SO_4 was increased, slope for OLS decreased drastically, whereas with the EIV models the decrease of the slope was moderate or negligible.

13AP.3

Filtration Efficiency and Discharging Behavior of Electret Filters. STEFAN SCHUMACHER, Rama Rao Jasti, Maximilian Kerner, Kilian Schmidt, Albert Hellmann, Sergiy Antonyuk, Christof Asbach, *Institut für Energie- und Umwelttechnik e.V. (IUTA)*

Electret filters find many applications since they offer a high initial filtration efficiency combined with a low pressure drop. They carry electric charges on the fibers, which interact either directly with charged particles by Coulomb attraction (electrophoresis), or by interaction with induced dipoles in both charged and uncharged particles (dielectrophoresis). However, a known drawback is that the efficiency of electret filters can drastically degrade with time due to exposure to particles, gases, solvents, or humidity.

In this study, the efficiency of electret filters with respect to differently charged aerosols was investigated to learn more about the charge and particle size dependence of the different electrostatic deposition mechanisms. Therefore, at first a unipolar diffusion charger was developed to provide highly negatively or positively charged particles. First experiments showed that the filtration efficiency strongly depends on the charge state of the particles. Furthermore, a pronounced discrepancy between measurements conducted with sodium chloride (NaCl) and di-ethyl-hexyl-sebacat (DEHS) is found, the origin of which has been further investigated.

To separate the electrostatic from the mechanical contributions, the filters were discharged with isopropyl alcohol (IPA) using two different techniques: On the one hand, the filters were immersed in liquid IPA, as applied for example in the European standard EN 779 for general ventilation filters. On the other hand, the filters were discharged in a cabinet (TDC 584, Topas GmbH) with IPA saturated air, as proposed by the new international standard ISO 16890, which replaces the EN 779 in 2018. Up to now, the comparability of the two methods is not well known. In our study, partially strong deviations in the efficiency of the two methods were found, the origin of which needs further investigation, but might have a strong impact on the reliability of the standards. Furthermore, we found that also for the discharged filters, charged particles are more efficiently deposited than neutral particles, hinting at the importance of image charge effects that are often neglected.

The experimental investigations are supported by 3D direct numerical simulation (DNS) of the filter media using the self-developed software DNSlab. Therefore, a realistic 3D model of the fiber structure is generated and differently charged areas are randomly distributed on the fiber surfaces to compare the effect of different charge configurations. The resulting electric field is computed by explicit integration of the fiber surface charges, while the flow field is obtained by numerical solution of the Navier-Stokes equations. Afterwards the trajectories of either unipolarly or bipolarly charged particles are tracked by the Lagrangian method considering all relevant forces. The corresponding filtration efficiency curves can be directly compared to the experimental results.

13AP.4

The Experimental Research on the Effect of Humidity on Fly-ash Collision Behaviour with Planar Surface. XUE LI, Ming Dong, Sufen Li, *Dalian University of Technology*

Particle dynamic processes are widely used in various industries, such as electrostatics precipitators (ESPs), fluidized beds, chemical and food. Especially agglomeration processes, particles interact with each other, deposition in low temperature ESPs. The discrete element modelling (DEM) is becoming a more commonly used tool for simulating dynamic processes involving solid particles. DEM traces the movement of all particles in a system and can provide particle-level information, which is often difficult to achieve by experiments. One of the required input parameters for DEM simulations is the coefficient of restitution, which can describe the energy losses during particle collisions and is important for proper modelling of particle dynamics.

In this present paper, a detailed research of particle-wall collision mechanics is proposed to determine the normal coefficient of restitution by using high-speed camera in different humidity conditions. Experiments were performed to measure the incident and rebound velocities of different kind of fly ash particles driven by gas flow onto a flat surface. The experimental system is designed for an aerosol inlet particle velocity range of 1 – 7 m/s. The coal used are bituminous coal from Fushun, Liaoning Province (LN), meager coal from Zhundong, Xinjiang Province (XJ), and anthracite coal from XinlinGol, Neimeng Province (NM) which are turned into fly-ash particles with a diameter of approximately 7 µm by using muffle furnace. The determination of the coefficient of restitution for single component particles is relatively straightforward process, however, when considering multicomponent particles like fly-ash and humidity environment, the unpredictable property of particles after impact makes the analysis of the coefficient of restitution more involved. In addition, a dynamic model is developed to calculate the damping coefficient, contact time, critical impact velocity, and contact displacement under both dry and humid conditions during impact. The modified Stokes number and elasticity parameter are proposed to further explore the relationship between the normal restitution coefficients under dry and humidity conditions. The main results can be summarized as follows.

Firstly, the results show that the normal coefficient of restitution decrease with increasing density, Young's modulus, and humid condition. The particles with humidity 65% seems much easier to be captured than other cases. These results demonstrate that the process of capture of micro-particle is more likely to happen for higher humidity.

Secondly, based on the dynamic model calculation, the damping coefficient and contact time are obtained with different impact velocities in a collision. The values of the damping coefficient and contact time are larger under humid conditions due to the effect of capillary force. The critical capture velocity increases with increasing humidity, because viscous damping by humidity increases.

Finally, the maximum contact displacement increases with normal incident velocity, and decreases with the humidity. The total force is a monotropic function of the contact displacement for the same kind of particle that is increasing with the contact displacement.

Keywords: Normal coefficient of restitution; Fly-ash; Humidity; Critical capture velocity

13AP.5

Investigation of Collisional Growth Rate of Titania Nanoparticles at High Flame Temperatures Through Molecular Dynamics Simulations. GIRISH SHARMA, Rajan K. Chakrabarty, Pratim Biswas, *Washington University in St Louis*

Nanoparticles are synthesized extensively using high-temperature flame and furnace aerosol reactors (1000-2200 K). At such high temperatures, the particles collide with each other and coagulate to form larger particles. Kinetic theory of gases is widely used to calculate the coagulation coefficient in the free molecular regime at high temperatures. This theory is verified both experimentally and through modeling, but only at ambient temperatures. Ideally, a correction factor accounting for the inter-particle forces should be incorporated. Previously reported modeling studies, performed at ambient temperatures, have shown that this correction factor can be greater or less than 1. This depends on the dominance of attractive or repulsive forces, which are material dependent. Moreover, at very high temperatures, nanoparticles have high thermal energy, and therefore instead of colliding and sticking, they can bounce back after collision, or even fragment the nanoparticle.

In this work, the aim is to investigate the coagulation correction factor for nanoparticle collisions for titania at high temperatures in free molecular regime. To achieve this, molecular dynamics (MD) simulations are performed. First, a realistic atomic model of the collision event for two titania nanoparticles is developed. Then, in the presence of interaction forces, particle trajectories are simulated over time. These different particle trajectories are then related to calculate the collisional correction factor. Following this, the effect of particle size, particle charge, functional groups, and particle temperature on collisional correction factor will be investigated. The insights on the physics of titania nanoparticle collisions, and the role played by interaction forces will be presented.

13AP.6

Effect of Time on Particle Resuspension from Substrates: Wind-tunnel Experiment and Analysis. Babak Nasr, JING QIAN, Morgan Minyard, Andrea R. Ferro, Goodarz Ahmadi, Suresh Dhaniyala, *Clarkson University*

Airflow-driven particle resuspension from surfaces plays an important role in indoor and outdoor air quality. The characteristics of particle removal from a substrate depend on particle size and morphology, substrate roughness, relative humidity, and flow field near the wall. The influence of these factors on the particle resuspension rates has been considered to varying extents in existing experiments and models. The current experimental studies, however, do not extensively account for the effect of time on article resuspension. In most resuspension processes, particles experience unsteady or intermittent airflow, and it is critical to consider the time-dependence of particle removal. In this study, set of wind-tunnel based particle resuspension experiments are conducted to evaluate the detachment fraction of particles as a function of time with controlled air flow. The influence of flow rate conditions -e.g., constant and stepping flow rate- on particle removal rate are investigated in our experiment focusing on micron-sized particles. Also, a semi-empirical model is described for time-dependent particle removal from surfaces exposed to turbulent flow. The model is derived based on a combination of experimental data reported in the literature and those obtained in our lab. In our presentation, we will describe the experimental procedure and the model development approach to validate the developed model.

13AP.7

Characteristics of Tire Wear Particles Generated by Tire Simulator under Various Driving Conditions. GIBAEK KIM, Seokhwan Lee, *Korea Institute of Machinery and Materials*

Traffic is known as an important contributor to particulate matter (PM) in urban areas. Traffic-related particles can be classified into exhaust and non-exhaust PM. Exhaust PM can be emitted by incomplete fuel combustion and lubricant volatilization. Non-exhaust PM can be generated through tire, brake, and road wear processes and road dust re-suspension. Due to the reduction of exhaust PM resulted from stringent emission regulations, the relative contribution of non-exhaust PM is expected to increase. Among the non-exhaust PM, tire wear particles (TWPs) have been less studied and have relatively high uncertainty in physical properties.

In this study, enclosing chamber (L: 3.5 m x W: 2.4 m x H: 2.2 m) equipped with the tire simulator and sampling systems were constructed to enable the detection of tire wear particles, thus excluding particles originated from other sources. The tire simulator can control load (100~8000 N), drum speed (20~180 km/h), tire speed (20~180 km/h), slip speed (-20~20 km/h), and tilt angle (-3~3°).

TWPs were directed to the sampling ports connected with several measurement devices. DustTrack DRX, aerodynamic particle sizer (APS), fast mobility particle sizer (FMPS) spectrometer, condensation particle counter (CPC), and optical particle counter (OPC) were employed to measure the physical properties of TWPs such as number concentrations, number size distributions, mass size distributions, and mass concentrations ($PM_{2.5}$ and PM_{10}). The results suggest that the physical properties of TWPs can vary with diverse driving conditions (load, tire speed, slip speed, and tilt angle) as well as types of tires and more experiments are being carried out.

13AP.8

New Insight into the Kinetics of Particle Resuspension Process. Jesica Gisele Benito, Rodolfo Omar Uñac, Irene Ippolito, ANA MARÍA VIDALES, *INFAP-CONICET, Universidad Nacional de San Luis*

Particle resuspension has been subject of special attention for researchers since many decades. This phenomenon is present in a wide range of fields, such as resuspension of airborne particles, reentrainment of sediments, human health, filtration systems, food industry and mining production.

In particle resuspension phenomena, experimental and simulation evidence demonstrate that air flow acceleration increases the velocity range needed for all the resuspension process. Nevertheless, this process becomes faster when acceleration increases.

Using a simple Monte Carlo model and, by analogy with the process of thermal desorption of molecules from surfaces, we are able to reproduce experimental data to analyze the main kinetic parameters of the problem. In our simulations, a monolayer of spherical particles are attached to the surface through an adhesion force that follows a Lognormal distribution and a Gaussian distribution is assumed for the aerodynamic forces. The stochastic process used for resuspension is based on the evaluation of probabilities depending on the ratio between the moments of the forces acting on each particle and using a Metropolis function.

To better understand the behavior related to the air flow acceleration used, we present a Kinetic Programmed Resuspension methodology, KPR, based on the analogy with the Temperature Programmed Desorption (TPD) technique. This technique enables us to obtain, through simple calculations, a transcendental equation that relates the friction velocity with the air flow acceleration and others particle-substrate constants.

Our numerical results are in agreement with the increase of particle rate with acceleration. Besides, the air velocity for maximum flow rate results to be higher as acceleration increases.

Finally, the KPR technique results in a potential tool which allows us obtaining particle-surface system constants by performing numerous repetitions of experiments for different values of air acceleration. This possible application could be devoted to find those parameters typically unknown in an experimental scenario.

13BA.1

Characterisation of Bioaerosols from Six Pig Farms Utilising Culture and Culture-Independent Methodologies. JOHN KERR WHITE, Jeppe Lund Nielsen, Anne Mette Madsen, *Aalborg University*

Farmers working with livestock are exposed to a mixture of different bacterial and fungal species in the form of bioaerosols. The microbial communities that compose these bioaerosols are known to be detrimental to workers' health and in some cases cause asthma and other airway maladies. Furthermore, pig farm workers often carry antibiotic resistant bacteria, such as methicillin-resistant *Staphyloccous aureus* (MRSA). MRSA is able to spread through the air in stables as a component of bioaerosols, and therefore it is crucial for workers' health to understand the level of exposure to potentially pathogenic microbes to help prevent disease.

During this study, amplicon sequencing of the bacterial 16S rRNA gene V4 region and the fungal ITS region using Illumina's MiSeq platform, as well as matrix-assisted laser desorption/ionisation time of flight mass spectroscopy (MALDI-TOF MS) were used for the identification of culturable, and non-culturable bacteria and fungi. Samples from from settling airborne dust were collected from pig farm stables of different types (care, farrowing, weaning, and slaughter) from different regions (Zealand, Jutland, and Funen) of Denmark. Electrostatic dust fall collectors (EDCs) were utilised for the collection of settling airborne dust from six swine farm stables. The settled dust was extracted from the cloths in an extraction buffer before being suspended in glycerol and frozen at -80°C until further use. Dilution series were made from 10^{-1} to 10^{-5} before being plated onto either nutrient agar or dichloran glycerol plates and incubated at 25°C and 10°C.

Culturing and identification by MALDI-TOF MS revealed a large diversity in bacterial and fungal species with *Aerococcus viridans*, *Staphylococcus equorum, Leuconostoc mesenteroides*, and *Staphylococcus saprophyticus* being the most dominant bacterial species. Interestingly, although *S. aureus* and MRSA had been previously detected when using selective media, they were not observed when samples were cultured on nutrient agar plates. This result could be due to lower concentrations of antibiotic resistant and non-resistant strains of *S. aureus* in comparison to other species, thereby masking the presence of antibiotic resistant and non-resistant *S. aureus*. Sequencing revealed a greater diversity of bacterial and fungal species when compared to MALDI-TOF MS analyses, with the most common bacterial species being members of the genera *Staphylococcus, Clostridium, Lactobacillus*, and *Turicibacter*. The most common fungal genera observed were *Debaryomyces, Alternaria*, and *Aspergillus*, whose members include known plant pathogens, possibly originating from the feed.

Inter- and intrafarm samples clustered differently in Principle Component Analysis (PCA) plots indicating that several small, but important, variables have an influence on the microflora in pig farms. The vast majority of the species identified are not considered human pathogens, but may contribute to the overall inflammatory potential of the dust.

This study highlights the need for multiple testing parameters to assess the full diversity of bacteria and fungi in environmental samples due to intrinsic limitations of different methods.

13BA.2

Size Distributions and Transport of Pathogenic Bioaerosol from Wastewater Treatment Plants. LIJIE LI, Xiao Huang, Hongliang Zhang, Michael Hoffmann, *California Institute of Technology*

Microbial pathogens transmitted by aerosols is a serious threat to public health as aerosols can transport in atmosphere and penetrate in human respiratory tract. Understanding the emissions and transport of pathogen-laden bioaerosol is of great importance in airborne infectious disease control. Wastewater treatment plants (WWTP) are fundamental facilities in urban environments and usually located in or adjacent to populated areas. Wastewater contains high concentrations of various microbial pathogens (e.g., pathogenic viruses, bacteria and protozoa) derived from human and animal wastes. Recent studies have found that the aerosolization of wastewater during the aerobic activated sludge treatment process produces a large amount of pathogenic bioaerosol, which can be transported hundreds of meters downwind. Therefore, WWTPs are a major source of pathogenic bioaerosol in urban area. The size distribution is the key parameter to determine the transport of bioaerosol in environment and human respiratory tract.

This work integrates the next-generation sequencing technique, high precision aerosol size differentiation instruments, and dispersion model to investigate the microbial composition, size distribution and transport of bioaerosol from WWTP. The aerosol number and volume distribution of total aerosol emission are measured online using an Aerodynamic Particle Sizer Spectrometer and Scanning Mobility Particle Sizer Spectrometer that include aerosols in the aerodynamic diameter from 10 nm to 10 µm. Size selected bioaerosols are collected near the aeration tanks for 4~5 hours at a local county sanitary district. The seasonal concentrations of total bacterial and bacteriophage MS2 extracted from sized aerosols are analyzed by real-time polymerase chain reaction (qPCR). The correlations between the distributions of microbe concentrations and aerosol number and volume are explored. Further, the microbial community structures and potential microbial pathogens associated with different sizes bioaerosol are analyzed by next-generation sequencing technique. The relationship between aerosol sizes and microbial composition as well as concentration is also discussed. By using the size distributions of aerosol number concentrations and microbe concentrations, the transport of potential pathogen riding on aerosol in atmosphere is predicted by the AERMOD dispersion model and the potential risk of bioaerosol exposure residents in nearby community is further evaluated by using International Committee for Radiological Protection (ICRP) lung deposition model. This work provides insights for the role of WWTP in pathogen transmission through airborne pathway.

13BA.3

Determining Distribution of Infectious Viruses in Aerosol Particles Using Water-Based Condensational Growth Technology. MAOHUA PAN, Leah Carol, John Lednicky, Arantzazu Eiguren Fernandez, Susanne Hering, Hugh Fan, Chang Yu Wu, *University of Florida*

Inhalation of virus aerosols can cause a wide range of adverse health effects and even severe casualties, depending on the species and distribution of the viruses in aerosol particles. The objective of this study was to determine the distribution of infectious viruses in airborne particles in the size range of 30 nm-300 nm, using bacteriophage MS2 as a surrogate for human viruses, with the newly introduced VIable Virus Aerosol Sampler (VIVAS). Aerosol particles containing MS2 bacteriophage were generated from a Collison nebulizer, conditioned by a dilution dryer, size selected by a differential mobility analyzer (DMA), and then collected by the VIVAS. Their physical size distributions were measured by a scanning mobility particle sizer (SMPS), while the counts of infectious viruses and the total viruses collected were quantified by the culture and quantitative reverse transcription-polymerase chain reaction (RT-qPCR) methods, respectively. For deionized (DI) water as the spraying medium, the amount of infectious and total viruses increased as particle size increased and reached the maximum at around 100 nm. This distribution pattern followed the aerosol's volume size distribution, instead of number size distribution. For Beef Extract (BE) and Artificial Saliva (AS), the same pattern following the aerosol's volume size distribution was observed. However, the number of infectious and total viruses per particle as a function of the particle size varied with the spraying medium: DI water approximated a cubic power scaling, AS approximated a quartic power scaling, and BE was between quadratic and cubic power scaling. A conceptual model was built to explain the different distribution patterns of viruses inside the particles - viruses could be homogeneously distributed or aggregated together inside or on the surface of the particles based on the hydrophilic/hydrophobic properties of the spraying media, resulting in different power scaling size distribution. Moreover, the survivability of MS2 with AS as the spraying medium was much higher than those with BE and DI water as the spraying media, suggesting that AS could provide better protection for MS2, which is likely due to the prevention of viable MS2 from reaching the air-water interface. Compared with prior studies that relied on assumed sampler efficiency, this study provides accurate assessment of the infectivity and transmissibility of airborne viruses for the first time without any such an assumption. Implication of the knowledge learned from this study could be very useful in guiding the design of an effective strategy to prevent the transmission of infectious virus aerosol, as viruses generated from different spraying media could end up with different sizes and transmitted through different pathways.

13BA.4

Reduction Strategies for Airborne Contaminants in Pre-Commercial Pig Buildings. VALÉRIE LÉTOURNEAU, Ariane Lévesque, Matthieu Girard, Stéphane Godbout, Stéphane.P Lemay, Caroline Duchaine, *IUCPQ-U.Laval, Canada*

Producers in Canadian pig buildings are exposed to large amounts of airborne contaminants. Gas, odors, dust and microbes (viruses, bacteria) in bioaerosols can be inhaled by workers as well as by surrounding rural communities from their environmental emission. Bioaerosols are generated from different sources: feed, litter, building materials, animals, and manure. Different strategies to reduce bioaerosols inside buildings (oil sprinkling, manure separation under a slatted floor) and environmental emissions (biotrickling filter) were investigated in two environmentally controlled rooms (16 animals per room). Animals were raised in one control room and in one test room in which reduction strategies were applied. One of the two seven week trials has been achieved. Ambient air of the control and test rooms was sampled as well as the upwind and downwind air of the biotrickling filter (isokinetic sampling with probes). PM10, PM2.5, PM4 (respirable), PM1 and bacteria were sampled on weeks 3, 5 and 6. A DustTrakTM DRX Aerosol Monitor (3 L/min, 10 min, Model 8534, TSI) allowed real-time mass readings of total dust, PM10, PM2.5 and PM1. Airborne bacteria were sampled into 15 mL of a phosphate buffered saline solution with a Coriolisμ Biological Air Sampler (200 L/min, 10 min, Bertin Corp.). From air samples, mesophilic bacteria were cultured on tryptic soy agar supplemented with 5 μg/mL of amphotericin. Preliminary results show a reduction of PM10, PM2.5, PM4 and PM1 inside the test room, ranging from 73% for PM10 to 65% for PM1. Moreover, concentrations of cultivable mesophilic bacteria were reduced by 92 ± 4% in the room where oil was sprinkled and manure separated. No reduction of airborne particles or cultivable bacteria was observed from the air coming out of the biotrickling filter. The unit was designed to reduce odours and gas (ammonia) by bacterial biofilms developing on a synthetic media and maintained biologically active by a continuously trickling nutrient solution. Bacterial diversity in upwind and downwind air samples will be evaluated by next generation sequencing to differentiate airborne test room-associated bacteria from those emitted. Total bacteria as well as specific human pathogenic agents such as Escherichia coli will also be quantified by PCR in air samples of the rooms and the biotrickling filter. Endotoxins will also be measured. The reduction strategies for airborne contaminants developed in the herein study are needed in the field as pig workers are still diagnosed with chronic bronchitis and asthma, and neighbouring farms are likely to be exposed to emitted pathogens that need to be controlled.

13BA.5

Bioaerosols Emissions from Open Waste Dumpsites: A case study of Olusosun Open Waste Dumpsite, Lagos Nigeria.

GODWIN AKPEIMEH, Louise Fletcher, Barbara Evans, *Member IPHEE, University of Leeds*

Introduction

In a bid to balance the high global rate of urbanization and the rate of municipal solid waste generation resulting from that urbanisation, the sustainable development goal (SDG) 11.6 aims to reduce the per capita environmental impact of cities by paying attention to air quality and municipal solid waste management. Unfortunately, most developing countries do not have the infrastructure to properly manage their municipal solid waste despite recording the highest rate of urbanization in the world. As a result, government authorities in these countries resort to open dumping as a cheap method for managing municipal solid waste. The bitter consequence of this is seen in the health and environmental impacts resulting from such treatment methods, one of which is bioaerosols emission.

Method

To assess the bioaerosols emission levels at open dumpsites, bioaerosol concentrations were measured at Olusosun open waste dumpsite, Lagos, Nigeria for 13 weeks. Air samples were collected across four points on the dumpsite using a six-stage Anderson sampler and an SKC Button sampler. Air samples were analyzed for total bacteria, gram-negative bacteria, Aspergillus fumigatus and total fungi.

Results

Gram-negative bacteria (Mean 1.6 × 103 CFU/m3, 310-3394 CFU/m3) showed the highest concentration as measured by the six-stage Anderson sampler and was followed by mesophilic bacteria (Mean 1.3 × 103 CFU/m3, 1.95× 102 - 3×103 CFU/m3), Total fungi (Mean 4.3×102 CFU/m3, 1.7-8.4 ×103 CFU/m3) and Aspergillus fumigatus (Mean 1.19 ×102 CFU/m3, 6× 100 -3.39× 102 CFU/m3). However, the result from the personal sampler indicated a higher bioaerosols exposure (100-1000 times more) from the activities they were engaged in, such as scavenging (gram-negative bacteria 3.0×106 CFU/m3, Total Bacteria 1.17 ×106, Aspergillus fumigatus 6.75 ×104); site monitoring (gram-negative bacteria 2.1×105 CFU/m3, Total Bacteria 6.0 ×105, Aspergillus fumigatus 3.0 ×105); waste sorting (gram-negative bacteria 1.74 ×106 CFU/m3, Total Bacteria 4.8 ×105, Aspergillus fumigatus 9.0 ×104). Analysing the participle size distribution, up to 77% of breathable particles emitted during dumpsite activities were within 0.65- 3.3 µm which could penetrate the lungs down to the alveoli.

Conclusion:

- Scavenging activity constitutes the highest exposure to bioaerosols as compared to other activities such as sorting and site monitoring (waste worker) carried out at open waste dumpsites.
- Gram-negative bacteria were higher across the dumpsite, which was also the highest pathogenic agent downwind of the dumpsite.
- The use of personal sampling and sampling with Anderson six-stage sampler, give better results on exposure levels as compared the Anderson six stage sampler alone as commonly used.

13BA.6

Systematic Characterization of the Wideband Integrated Bioaerosol Sensor (WIBS), Including Fluorescence Thresholding and Clustering Analysis Strategies. NICOLE SAVAGE, Christine Krentz, Tobias Könemann, Taewon Han, Gediminas Mainelis, Christopher Pöhlker, J. Alex Huffman, *University of Denver, now at Aerosol Devices*

There has been a recent steep increase in the frequency of published studies utilizing commercial instrumentation based on ultraviolet laser/light-induced fluorescence (UV-LIF) for detection of bioaerosols both outdoors and in the built environment. Significant work over several decades supported the development of the general technologies, but efforts to systematically characterize the operation of new commercial sensors has remained lacking. Specifically, there have been gaps in the understanding of how different classes of biological and non-biological particles can influence the detection ability of LIF-instrumentation.

We will present a summary of two recently published papers [1,2] that have systematically characterized the wideband integrated bioaerosol sensor (WIBS-4A) instrument and whose conclusions can be broadly applied regarding other commercial UV-LIF bioaerosol sensors. The laboratory study used 69 types of aerosol materials, including a representative list of pollen, fungal spores, and bacteria as well as the most important groups of non-biological materials reported to exhibit interfering fluorescent properties [1]. We will highlight the importance that particle size plays on observed fluorescence properties and will also discuss several particle analysis strategies, including the commonly used fluorescence threshold defined as the mean instrument background (forced trigger; FT) plus 3 standard deviations (σ) of the measurement. Changing the particle fluorescence threshold was shown to have a significant impact on fluorescence fraction and particle type classification. We conclude that raising the fluorescence threshold from FT + 3σ to FT + 9σ does little to reduce the relative fraction of biological material considered fluorescent, but can significantly reduce the interference from mineral dust and other non-biological aerosols. In particular, we examined several classes of highly fluorescent interfering particles, including examples of brown carbon, diesel soot, and cotton fibers, and we will discuss how these may impact WIBS analysis and data interpretation in various indoor and outdoor environments.

Results of the systematic laboratory study were analyzed using a hierarchical agglomerative clustering (HAC) algorithm applied to WIBS data in a similar way as recently used by the team at the University of Manchester (e.g. [3]). We systematically investigated 19 one-on-one matchups of individual particles types and varied input parameters in order to optimize clustering quality and also tested scenarios suggested in the first paper [1] regarding fluorescence thresholding strategies. Finally, we tested the clustering methods against several synthetic mixtures of laboratory particles in order to understand possible limits to the HAC strategy and to understand how the analysis techniques can best be applied to complex real-world data.

An overview of the main conclusions from these two papers will be presented. The studies were designed to propose analysis strategies that may be useful to the broader community of UV-LIF instrumentation users in order to promote deeper discussions about how best to continue improving UV-LIF instrumentation and analysis strategies.

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13BA.7

Using Single Particle Fluorescence to Characterise Bioaerosols Emissions from Green Waste Composting. ZAHEER AHMAD NASIR, Sean Tyrrel, *Cranfield University, MK43 0AL, UK*

The potential public health risks from bioaerosols emissions due to increasing waste management facilities, such as open windrow composting, is a growing concern. However, the emissions from such processes are poorly characterised mainly due to the limitations in currently used sampling and analysis methods which offer snapshot data with low temporal resolution. Recent advancement in bioaerosols detection and characterisation technologies, for example, fluorescence spectroscopy offer the capability to monitor bioaerosols in real time and can significantly advance the existing state of knowledge on nature and magnitude of emissions from such facilities. But the broad fluorescence emission detection bands in existing instruments hinder to resolve spectrally integrated signals from the biological fluorophore. The single particle dual excitation multiple fluorescence band systems can offer highly resolved spectral information improving measurement selectivity and classification strategy. This study aims to detect and characterise bioaerosols emissions in real time from green waste composting by using a novel light-induced fluorescence sensor with highly resolved fluorescence intensity measurements (Spectral Intensity Bioaerosol Sensor – SIBS, Droplet Measurement Technologies, USA). The SIBS records a range of data (size, shape, and fluorescence emission across 16 wavelength bands from 288 - 735 nm for two excitation wavelengths (280 nm and 370 nm) on single particles in real time. Four measurements during daytime were carried out between October – December 2016 by using the SIBS downwind of the source at a green waste composting facility. There was considerable temporal variability in the concentration of total and fluorescent particles during different operational activities. Turning of windrows led to higher concentrations of particles in comparison to screening and shredding. There was a shift towards larger size particles during activities. A shift in the MMAD of fluorescent particles was observed during activity and no activity periods. During no activity (no screening and turning) the MMAD for fluorescent particles was 0.66 µm and during activity, the MMAD of fluorescent particles increased to 5.57 µm. In terms of fluorescence spectra, differences were found in the general shapes of the emissions spectra during activity and no activity periods. The SIBS provides additional spectral information in comparison to instruments based on broad emission bands. However, assignment of fluorescence to atmospherically relevant biological fluorophore is challenging and further lab-based studies are needed to interpret the resolved emission spectra recorded by the SIBS. Simultaneously numerical methods and tools are needed to analyse big data to develop discrimination algorithms.

13BA.8

Identification and Atmospheric Abundance of Primary Biological Aerosol Particles. Maria Zawadowicz, Karl D. Froyd, Daniel Murphy, Dominick Spracklen, Colette Heald, Peter Buseck, DANIEL CZICZO, *MIT*

Measurements of bioaerosol (primary biological aerosol particles and particles containing fragments as part of an internal mixture), especially in the free troposphere, are scarce. Single particle mass spectrometry (SPMS) has been used to probe aerosol chemical composition from ground and aircraft for over 20 years. We present a method for identifying bioaerosols using SPMS. We show that identification of bioaerosol using SPMS is complicated because phosphorus-bearing mineral dust and phosphorus-rich combustion by-products such as fly ash produce mass spectra with peaks similar to those typically used as markers for bioaerosol. We have developed a methodology to differentiate and identify bioaerosol using machine learning statistical techniques applied to mass spectra of known particle types. This improved method provides far fewer false positives compared to approaches reported in the literature. The new method was then applied to ambient data sets, showing an abundance 10 or more times lower than for mineral dust. The methodology extends measurement of bioaerosol using historic data, allows for comparison to modern techniques, and is in general agreement with a global aerosol model.

13CA.1

Chemical Characterization of Biomass Burning Aerosols: Can We Reduce the Complexity of Primary Aerosol Emissions? ALESSANDRO FRANCHIN, Ann M. Middlebrook, Gabriela Adler, Matthew Coggon, Joost de Gouw, Jessica Gilman, Abigail Koss, Jesse Kroll, Kara D. Lamb, Christopher Lim, James Roberts, Joshua P. Schwarz, Kanako Sekimoto, Vanessa Selimovic, Chelsea Stockwell, Nick Wagner, Carsten Warneke, Rebecca Washenfelder, Caroline Womack, Robert J. Yokelson, Bin Yuan, *CU CIRES - NOAA ESRL*

Aerosols emitted by fires influence the Earth's radiative budget and play a key role in degrading air quality. Their effects range from a local to a global scales. In the near future, drier conditions and an increase in average temperatures will very likely increase the frequency and magnitude of wild fires. Despite a large effort by the scientific community, aerosols emitted by open-burning fires are still not completely understood and characterized. The challenges are related to the complexity and variability of emissions. In fact, biomass-burning emissions show great differences depending on fire and environmental conditions, fuel type, and aging of the plume.

With our study, we analyze an extensive set of laboratory burns with the goal of understanding, and possibly reducing this complexity. We show the time-resolved chemical composition of the aerosols generated by laboratory fires during the NOAA 2016 FIREX measurement campaign at the Missoula Fire Science Laboratory. During the campaign, we sampled emissions from more than 35 different fuels relevant for the Western United States using an Aerosol Mass Spectrometer at high time resolution (<1 s). We show how the chemical composition of the biomass-burning aerosol changes in different phases of the fire for different burns. We highlight similarities and differences between different fuels, different stages of the fires and different fuel type (e.g., canopy vs. litter vs. duff). We compare our results with the results obtained by using a positive matrix factorization analysis for the gas phase volatile organic compounds, with an attempt to link the gas phase to the aerosol phase emissions. Finally, we compare the time-resolved and the fire-integrated results. Our final aim is to provide tools for a better parametrization of primary emissions from biomass burning.

13CA.2

Chemical Composition of Biomass Burning Particles Measured with a Soot Particle Aerosol Mass Spectrometer Downwind during the BBOP Study. TIMOTHY ONASCH, Anita Avery, John Shilling, Joda Wormhoudt, Arthur J. Sedlacek, Edward Fortner, Mikhail Pekour, Shan Zhou, Sonya Collier, Qi Zhang, Lawrence Kleinman, Ernie R. Lewis, Andrew Freedman, Leah Williams, *Aerodyne Research, Inc.*

The Biomass Burning Observation Project (BBOP), a Department of Energy (DOE) sponsored field campaign, measured emissions from wildland fires in the Pacific Northwest and agricultural burns in the Central Southeastern US from the DOE Gulfstream-1 airborne platform over a four month period in 2013. Rapid physical, chemical and optical changes in biomass burning particles were measured downwind (< 3 hours temporally) from wildland fires.

The chemical composition of the particulate emissions was characterized using an Aerodyne Soot Particle Aerosol Mass Spectrometer (SP-AMS) and will be presented in the context of the fire location, combustion conditions, and optical property measurements, including extinction and single scattering albedos. The SP-AMS was operated with both laser and resistively heated tungsten vaporizers, alternating between laser off and on. With the laser vaporizer off, the instrument operated as a standard high resolution AMS. With the laser vaporizer on, the SP-AMS was also sensitive to the refractory black carbon (rBC) content, in addition to the non-refractory components. Results from both vaporizer configurations will be presented and contrasted.

Chemical signatures indicate different combustion conditions within a given fire plume, implying a high diversity within a given burn. The non-refractory chemical composition, including the level of oxidation, i.e., O:C, H:C, and organic mass/organic carbon ratios (OM:OC), changes systematically during the hours of atmospheric transport before measurement. The oxidation of the organic compounds increases with downwind advection, while the primary markers, such as m/z 60, decrease. These chemical changes appear to continue downwind, when compared with additional further downwind measurements, even as the ratio of organic mass to carbon monoxide appears to remain constant. We will also discuss the chemistry in light of observations of tar ball formation and evolution, including results from laboratory studies on tar balls.

13CA.3

The Effect of Hydrophobic Glassy Organic Material on the Cloud Condensation Nuclei Activity of Internally Mixed Particles with Different Particle Morphologies. Ankit Tandon, Nicholas Rothfuss, MARKUS PETTERS, *North Carolina State University*

Particles composed of organic and inorganic components can assume core-shell morphologies. Previous studies have shown that hydrophobic organic shells can slow water vapor diffusion into the particle core. The kinetic limitation of water uptake may increase the critical supersaturation required to activate such particles into cloud droplets. Here we test this hypothesis through laboratory experiments. Polyethylene was used as proxy for a hydrophobic glassy organic material. Temperature dependent viscosity and cloud condensation nuclei (CCN) activity of the polyethylene were measured. Results show that the viscosity of 50 nm polyethylene particles is 5×10^6 Pa·s at ~61°C. Extrapolation of the temperature dependent viscosity indicates that the particles are glassy at room temperature. Polyethylene particles were inactive as CCN at diameters less than 300 nm at 1% water supersaturation. Ammonium sulfate was used as proxy for CCN active inorganic material. Internally mixed particles were generated using coagulation of oppositely charged particles; charge-neutral polyethylene-ammonium sulfate dimers were then isolated for online observation. Morphology of these dimers was then varied by partially or completely melting the polyethylene such that the liquefied polyethylene partially or completely engulfed the ammonium sulfate. Critical supersaturation was measured as a function of dry particle volume, particle morphology, and organic volume fraction. Our results show that kinetic limitations do not change the critical supersaturation for particles composed of equal volumes of polyethylene and ammonium sulfate. Water transfer will be less hindered in hydrophilic glassy organic materials due to the plasticizing effect of water on dissolving organic compounds. Based on extensive evidence from literature data, hydrophobic glassy organic materials are likely not prevalent in the atmosphere. Furthermore, timescales of humidification are shorter in CCN instruments than in atmospheric updrafts. Therefore, our experiments suggest that, near laboratory temperatures, mass transfer limitation by glassy organic shells is unlikely to affect cloud droplet activation.

13CA.4

Quantification of Fossil and Non-Fossil SOA from Combined 14C/AMS-PMF Analysis for the SOAS Field Campaign.

SOENKE SZIDAT, Matthias Vonwiller, Gary Salazar, Weiwei Hu, Jose-Luis Jimenez, Eric Edgerton, Stephanie L. Shaw, Andre S.H. Prévôt, *University of Bern*

The Southern Oxidant and Aerosol Study (SOAS) was a large field campaign during June-July 2013 in the southeast USA (Hidy et al., 2014; Hu et al., 2015; Carlton et al., 2018). Vast forested areas emitting large amounts of organic compounds and proximity to metropolitan areas present an ideal environment to investigate the influence of anthropogenic emissions on the biogenic secondary organic aerosol (SOA) formation. The main site of this study, located in rural Centreville, AL, was equipped with a wide variety of state-of-the-art analytical instruments. This project focuses on the source apportionment of the organic carbon (OC) fraction of ambient aerosol samples, through combination of radiocarbon (^{14}C) data with positive matrix factorization information from online aerosol mass spectrometry measurements (AMS-PMF).

Analysis of the long-lived radioactive isotope ^{14}C is a unique source apportionment tool: it unambiguously separates fossil from non-fossil sources, as ^{14}C has completely decayed in fossil fuels, whereas modern materials have the contemporary radiocarbon level (Szidat, 2009). ^{14}C was measured for total carbon (TC) and elemental carbon (EC) (Zhang et al., 2012) from quartz filters that were collected at Centreville with daily resolution. This allowed the apportionment of fossil vs. non-fossil sources for EC and OC. Although OC mainly originated from non-fossil sources, a certain fraction was attributed to emissions from fossil sources. These results were compared with AMS-PMF data from a high-resolution time-of-flight AMS (Hu et al., 2015), which identified six different factors, i.e. biomass burning organic aerosol (BBOA), SOA formed through direct condensation of low-volatility oxidation products from isoprene (ISOPOOH-SOA), isoprene epoxydiols-derived SOA (IEPOX-SOA), low-oxidized oxygenated organic aerosol I, attributed to mostly biogenic sources (LO OOAI), low-oxidized OOA II, attributed mostly to anthropogenic sources (LO-OOAII) and more-oxidized OOA (MO-OOA). On average, the less well-understood fractions LO-OOAI, LO-OOAII and MO-OOA comprise ~3/4 of the total organic aerosol mass. ^{14}C analysis of EC enables the distinction of sources of this carbonaceous aerosol fraction between fossil-fuel combustion (mainly from traffic) and biomass burning. It indicated a larger contribution from biomass burning compared to other source apportionment techniques or results from bottom-up emission inventories.

The combination of ^{14}C and AMS-PMF analysis provides the potential to apportion fossil vs. non-fossil sources for components for which the non-fossil fraction cannot by analyzed directly, such as SOA (Zotter et al., 2014). In this work, we present such results for the SOAS campaign based on Markov chain Monte Carlo calculations to gain more insight into the sources of SOA precursors. LO-OOAI, LO-OOAII and MO-OOA reveal different contributions of fossil and non-fossil sources, which allows a better understanding of these AMS-PMF factors.

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13CA.5

Discrepancies Between the Volatility Distributions of OA in the Ambient Atmosphere and the Laboratory. Eleni Karnezi, Evangelos Louvaris, Evangelia Kostenidou, Kalliopi Florou, Kerrigan Cain, SPYROS PANDIS, *Carnegie Mellon University, University of Patras*

Organic compounds represent a significant fraction of submicrometer atmospheric aerosol mass. Even if most of these compounds are semi-volatile in atmospheric concentrations, the ambient organic aerosol volatility is quite uncertain. This work attempts to synthesize the organic aerosol volatility distribution estimates in both ambient and laboratory studies and quantifies the role of other properties that affect volatility estimates such as the vaporization enthalpy and accommodation coefficient that are usually assumed.

Measurements combining a thermodenuder (TD) and a High Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS) that took place in Paris (summer 2009 and winter 2010), Athens (winter 2013) and Finokalia (summer of 2016) are used for the analysis. These are combined with similar measurements of both primary and secondary organic aerosol (cooking OA and SOA, SOA from VOCs) that took place in the smog chambers of the Institute of Chemical Engineering Sciences in Patras and Carnegie Mellon University in Pittsburgh. The Karnezi et al. (2014) method is applied to these datasets in order to estimate the volatility distribution together with the vaporization enthalpy and the accommodation coefficient for the organic aerosol (OA) and its components (based on positive matrix factorization).

Our results suggest that the laboratory OA is significantly more volatile than the ambient from the same source or precursor. However, a significant part of this discrepancy is due to the different OA concentration levels present in the two types of studies. At the high concentration levels present in the laboratory the semivolatile components with higher volatility partition into the particle phase and the OA becomes more volatile (Donahue et al., 2006). The volatility basis set framework can be used to estimate the volatility distribution of the laboratory aerosol at ambient concentration levels allowing a direct comparison of the two distributions. This technique is applied to all the data sets. The results suggest that the gap is a lot smaller than originally thought. For example, for cooking OA the ambient and laboratory volatilities are practically the same when compared at the ambient concentration levels of a few micrograms per cubic meter. The differences of the volatility distributions of the various OA components determined during the PMF analysis of the AMS measurements at the same factor concentration levels are also lower. These volatility differences can be related to differences in the AMS spectra of the various factors and are probably due to the source mix or the degree of atmospheric processing in each study. The vaporization enthalpies of the OA factors were relatively consistent across the different campaigns examined and the model suggests small mass transfer resistances in most cases.

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13CA.6

Prediction of Atmospheric Organic Aerosol Concentrations From Carbonyl Absorption in the Mid-Infrared. Matteo Reggente, Robin Modini, Giulia Ruggeri, SATOSHI TAKAHAMA, Andrew Weakley, Alexandra Boris, Ann Dillner, Provat Saha, Andrew Grieshop, Christoph Hueglin, Christopher Pöhlker, Meinrat O. Andreae, Samara Carbone, Paulo Artaxo, *EPFL*

Fourier Transform-Infrared (FT-IR) spectra of particulate matter is chemically informative with regards to molecular bonds and functional groups present in the sample. The process of building calibration models for various PM constituents (e.g., functional groups, carbon content) allows us to extract useful features for quantitative prediction, and inform us regarding the most explanatory vibrational modes (Dillner and Takahama 2015, Takahama et al. 2016).

We develop a new algorithm for eliminating uninformative wavelengths in spectroscopic calibration for prediction of organic carbon (OC) concentrations equivalent to that of thermal optical reflectance (TOR) measurements. Using this algorithm together with FT-IR spectra obtained from Teflon filters and TOR OC concentrations measured from collocated quartz fiber filters in 526 samples from 7 sites in the US IMPROVE monitoring network for 2011, we build a calibration model that accurately predicts TOR-equivalent OC mass concentrations in $PM_{2.5}$ for more than two thousand samples collected across the same sites in 2011 and 11 additional sites in 2013. Surprisingly, this model uses 10 wavelengths spanning a very narrow region of ~0.6 micrometers in the mid-infrared region. Investigation with reference compounds in laboratory-generated aerosols suggests that this region is not associated with hydrocarbon C-H structures, which is typically prominent in atmospheric PM (more than 50% by mass in IMPROVE network samples; Ruthenburg et al. 2014). However, we find strong association with carboxylic acids, and weaker but non-negligible association with ketonic carbonyls. We further find that these 10 wavelengths can be used to predict PM2.5 thermal optical transmittance (TOT) OC in PM2.5 in Zurich, Switzerland, and submicron OM in the Amazon rainforest, Brazil, (GoAmazon campaign) and Centreville, Alabama, USA (Southern Oxidant and Aerosol Study campaign). We discuss further interpretation of this model and implications for organic aerosol modeling.

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13CA.7

Optical Properties of Biomass Burning Carbonaceous Aerosol from Controlled Laboratory Burns and Ambient Wildfires. DIAN ROMONOSKY, Samantha Gomez, Jared Lam, Christian Carrico, Allison Aiken, Petr Chylek, Thom Rahn, Manvendra Dubey, *Los Alamos National Lab*

Biomass burning and wildfires are important regional sources of particles and trace gases that degrade air quality, visibility, and impact climate. Light absorbing carbonaceous aerosol (LACA) and light scattering carbonaceous aerosol (LSCA) are major components of these optically complex emissions. The most absorbing class of LACA is refractory-LACA (r-LACA), commonly referred to as soot. Another component of LACA includes brown carbon (BrC), which is formed in the atmosphere, is non-refractory (nr-LACA), and has steeper absorption at shorter wavelengths than r-LACA. Both r-LACA and nr-LACA from biomass burning sources contribute to atmospheric warming. However, different processes control the amount of r-LACA and nr-LACA that are emitted and their evolution in the atmosphere, which determines the aerosol properties. These processes include fuel composition and combustion phase in the near field as well as the water affinity, volatility and photochemical processes in the far field. To better understand the optical properties of biomass burning aerosol, laboratory studies of smoke emissions were conducted in the Center for Aerosol Experiments (CAFÉ), at Los Alamos National Laboratory. The focus was on both native and invasive species found in the Southwestern U.S. to examine the influence fuel type and combustion conditions had on biomass burning emissions. During this time, ambient events were also measured at CAFÉ, including the El Cajete/Bonita wildfire (June 2017) and the Jemez/Valles Caldera prescribed burns (October 2017). Here we report and analyze single scattering albedo (SSA), absorption angstrom exponent (AAE), and mass absorption coefficient (MAC) values from the laboratory burns and wildfire events. Preliminary results show our laboratory burns produced aerosol with a wide range of optical properties, with some producing more strongly light-absorbing particles (SSA at 405 nm = 0.4-0.5) and others producing weakly light absorbing particles (SSA at 405 nm ≈1). AAE (405/780 nm) ranged from 1, indicative of r-LACA, to 4.5, suggesting the presence of nr-LACA during flaming and smoldering combustion phases. MACs for r-LACA show variability attributed to mixing state changes. The variability in our laboratory burns was found to be greater than in ambient fires, indicating a confluence of optical properties for ambient aged aerosol in comparison to the near-field laboratory emissions. We will present direct measurements of MACs of organic aerosol (including LACA and LSCA) using our SP-AMS. Mie theory calculations constrained by observed size distributions are used to interpret the optical properties of the smoke. Our results will gain insights into fundamental processes controlling the optical properties of biomass burning smoke and explain its variability to better predict their impact on climate.

13CA.8

Estimates of Radiative Forcing by Carbonaceous Aerosols over Northern India. A.S. Panicker, R. Aditi, G. BEIG, K. Ali, *IITM, Pune, India*

Sampling of $PM_{2.5}$ particles over two Northern Indian Cities (Jabalpur (JBL) and Udaipur (UDPR)) were carried out during November 2011-November 2012 (up to September 2012 over UDPR). An advanced DRI Thermal optical carbon Analyzer was used to extract the Elemental Carbon (EC) and Organic Carbon (OC) using Impove_A protocol from the sampled filter papers. The elemental carbon concentrations were up to 7.36 ± 1.99 µgm^{-3} over JBL and were as high as 10.78 ± 4.85 µgm^{-3} over UDPR. Whereas the corresponding OC concentrations showed much larger concentration in different seasons (as high as 19.37±12.6 µgm^{-3} over JBL and was up to 39.71±13.05 µgm^{-3}over UDPR). The radiative forcing for OC and EC has been estimated using Optical properties of Aerosols and Clouds (OPAC) model along with a radiative transfer model (Santa Barbara Discrete Ordinate Radiative transfer Model). The surface forcing for OC found to be -1.99 ± 0.99 Wm^{-2} to -2.76± 1.96 Wm^{-2} over JBL and -1.36± 1.06 Wm-2 to -4.67 ± 1.76 Wm^{-2} over UDPR. The Top of the Atmosphere (TOA) forcing values found to be -0.53 ±0.39Wm^{-2} to -1.50± 0.70Wm^{-2} over JBL and -0.75 ± 0.59 Wm^{-2} to -2.07 ± 1.35 Wm^{-2} over UDPR. However the magnitude of EC forcing found to be more than ten fold higher than OC forcing (As high as -20.10 Wm^{-2} at surface and +9.1Wm^{-2} at TOA over JBL and -34.35 Wm^{-2} at surface and + 12.51 Wm^{-2} at TOA over UDPR) due to its strong atmospheric absorption, inspite of much lower concentration compared to OC.

Key words: Organic Carbon, Elemental Carbon, radiative forcing

13CB.1

A Study on Emission Characteristics of Indian and Chinese Coal. RANJIT KUMAR, He Jing, Pratim Biswas, *DEI, Daya*

Coal is an important source of energy and it will remain important to meet the world energy demand. The present study investigates the emissions from combustion of Indian coal and Chinese coal in different combustion conditions. The mass concentration, number concentration, size distribution and surface area concentration in alveolar and tracheobronchial regions were determined using DutTrak, SMPS and AeroTrak respectively, in the fly ash of coal combustion. The mass concentration of PM1, PM2.5 and PM10, and surface area concentration of emission particle from coal combustion were critically higher. PM1, PM2.5 and PM10, emission concentration was higher from Chinese coal in comparison to Indian coal. The number size distribution revealed unimodal distribution. The high surface area concentration of particles implies greater exposure and has health implications.

13CB.2

Does Coal Combustion Emit Siloxane? ZHAOJIN AN, Wei Zhou, Haixia Ren, Mo Xue, Jianguo Deng, Jingkun Jiang, *Tsinghua University*

Siloxane is a type of organic polymer widely used in industries for its good thermostability and chemical resistance. It has been reported that siloxane exists in aerosols sampled from ambient air, indoor air, and other sources. Siloxane emitted from carbon conductive silicone tube caused aircrafts in aerosol sampling (Timko et al. 2009, Yu et al. 2009). Siloxane in ambient air samples (Hayden et al. 2008) and coal combustion samples (Schneider et al. 2006) were usually attributed to silicone materials used in the sampling system. In this study, three coal types (bituminous, anthracite, and semicoke coals) were burned in a household stove (NS18-17, 18 kW; Laowan Company; Beijing, China) for heating and cooking. A quartz filter based comprehensive two-dimensional thermal desorption aerosol GC/MS (QF-2D-TAG) were to characterize siloxane emission. A home-made particle size distribution measurement system (PSD) (Liu et al. 2016) was used to measure aerosol in the range of 3 nm to 10 µm. Carbon monoxide and carbon dioxide were monitored to estimate the combustion efficiency of the stove.

In the QF-2D-TAG, organic aerosol was first sampled by the quartz filter in the collection and thermal desorption (CTD) cell. The sample was then heated to 300°C and delivered into the first dimension column for separation based on their boiling points, and a modulator periodically trapped analytes eluting from the first column, and periodically released them into the second column for separation based on their polarity. In-situ hourly measurement of molecular level organic species was realized. Compared to the first thermal desorption aerosol GC/MS-FID (TAG) (Williams et al. 2006) and SV-TAG (Zhao et al. 2013) for measuring semi-volatile compounds, a quartz filter based CTD cell and a comprehensive two-dimensional modulator was used for the QF-2D-TAG.

Molecular level siloxane was measured during a complete residential coal combustion process. Siloxane were largely detected in ignition and fierce combustion stages (Zhou et al. 2016) and $(SiOC_2H_6)_6$ was one of the most abundant species. More siloxane was detected at higher combustion temperature. Only metal tubing was used in the coal combustion system and the sampling and measurement system to avoid artifacts from carbon tubing.

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13CB.3

Effects of Pressure and Coal Seams on the Characteristics of Coal Fly Ash and Submicrometer Particle Size Distribution.

ZEHUA WANG, Zhichao Li, Shuhua Ma, Shili Zheng, Pratim Biswas, *Washington University in St Louis*

Coal combustion accounts for 33% of the total electricity generation in the US and both greater than 70% in China and India (Biswas et al. 2011; Wang et al. 2013). In addition, China, USA and India are the top three countries in coal consumption worldwide (Yao et al. 2015). As a result, large amounts of fly ash in the exhaust gas of coal combustors are collected at coal-fired power plants and poses challenges for appropriate disposal and re-utilization. In the meantime, large numbers of hazardous submicrometer particles are emitted to the ambient air due to their high penetration in conventional particle control devices. To effectively achieve either reuse or capture of fly ash, it is imperative to characterize fly ash using a holistic approach. Moreover, coal combustion is also one of the main source of carbon dioxide emission. The pressurized oxy-combustion, which can increase the efficiency and reduce the cost for the carbon dioxide capture and storage or utilization, is considered as a promising alternative to the traditional coal combustion (Gopan et al. 2014).

This study is focused on investigating the effects of pressure and coal seams on the characteristics of the coal fly ash and the submicrometer particle size distribution. Fly ash was produced by combustion of different coals from the US, India, and China in a lab-scale drop-tube furnace at different pressure. The submicrometer particle size distributions, mineralogy, and surface area of the generated fly ashes were characterized using a scanning mobility particle sizer (SMPS), x-ray diffraction (XRD), and Brunauer-Emmett-Teller (BET), respectively. The morphology and chemical composition were examined using a scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDX). The results indicate that the US PRB coal fly ash was mainly composed of quartz, anhydrite, lime and hematite, while both India Chandrapur and China S02 coal fly ash were mainly composed of quartz and mullite. However, India Chandrapur coal fly ash had higher silicon content, while China S02 coal fly ash was rich in alumina. With an increase in pressure, the concentration of submicrometer particles was reduced. This study is meaningful to understanding the characteristics of coal fly ash generated from the pressurized combustion system, which can thus provide insights for more effective capture of submicrometer particles in pressurized particle collection devices.

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13CB.4

Black Carbon Emissions Using Marine Fuels: An Instrument Comparison and Emissions Characterization. STEPHANIE GAGNE, Brigitte Behrends, Ali Momenimovahed, Kevin Thomson, Gert Jakobi, Volker Wichmann, *National Research Council Canada*

The International Maritime Organization (IMO) is investigating measurement methods to assess the climate impact of Black Carbon (BC) from international shipping in the Arctic. BC emissions from marine engines have very different properties compared to other transportation sectors. The fuels used generally contain more sulphur, ash, and a higher fraction of organic components, especially (but not limited to) when using Heavy Fuel Oil (HFO). The engine technology varies widely and a whole range of fuels are used including Liquefied Natural Gas, Diesel, HFO and blends. All these factors influence the detection of BC by the different instruments, and complicate their calibration.

In a measurement campaign held in Rostock, Germany in the summer of 2016, we measured BC emissions from a one-cylinder research engine, burning three different marine fuels, and varying the engine load. We used 6 different BC mass concentration measurement techniques: a Droplet Measurement Technology Photo Acoustic eXtinctiometer (PAX), two Artium LII300 (Laser-Induced Incandescence, LII), a Sunset Laboratory Thermal-Optical Analyzer (TOA, using transmittance and reflectance), an AVL 415SE Smoke Meter, an AVL MicroSoot Sensor (MSS), and a Magee Scientific Aethalometer. We also gathered ancillary information on the emitted particles such as by TEM images, EDX analysis, and effective density measurements with and without a denuder.

In this work, we present how BC emissions varied for different fuels and different engine loads. We also analyze the variation in the response of different BC instruments depending on their measurement principles and the emissions properties at different test points. We find that the fraction of organic material influences the degree to which the instruments agree. We also discuss what influence the presence of ash may have on the different instruments.

13CB.5

Infrared-Absorbing Carbonaceous Tar Can Dominate Light Absorption in Heavy-Fuel-Oil PM. JOEL CORBIN, Hendryk Czech, Dario Massabò, Carlo Mennucci, Francesco Buatier de Mongeot, Gert Jakobi, Fengshan Liu, Prem Lobo, Amewu Mensah, Jürgen Orasche, Simone Pieber, Benjamin Stengel, Li-Lin Tay, Marco Zanatta, Ralf Zimmermann, Andre S.H. Prévôt, Imad El Haddad, Martin Gysel, *Paul Scherrer Institute*

Heavy fuel oil (HFO) is widely used in the open ocean and Arctic, and is known to emit substantial amounts of black carbon and polyaromatic hydrocarbons. However, we show here that those light-absorbing species do not consistently comprise the bulk of the direct climate forcing by HFO emissions. Our characterization of a marine engine shows that a previously unidentified particle type, insoluble and infrared-absorbing tar, dominates total light absorption at low engine loads. Tar particles have a higher fraction of sp^3-bonded carbon than BC, and consequently a high Angstrom absorption exponent (AAE) of ~2.0 at wavelengths 370–1000nm. As this tar is refractory, thermal–optical analysis cannot be used to distinguish it from BC; its climate effects are most accurately quantified by direct light-absorption measurements taken at specific wavelengths. Field observations suggest that tar already contributes to accelerated Arctic snow melt, an effect which may be magnified as Arctic shipping continues to intensify.

13CB.6

Jet Engine Exhaust at the Airport – HRTEM and XPS Analyses. RANDY VANDER WAL, Chung-Hsuan Huang, *Penn State University*

Few studies of aircraft and ground support equipment on airport and regional air quality exist. Transmission electron microscopy (TEM) of jet exhaust particulate matter can provide a direct measure of particle size and their change with respect to engine power. Of particular concern are the innumerable small particles, consisting of organic carbon produced at idle conditions. These likely arise as secondary organic aerosols as a result of volatile condensation. Such particles of < 20 nm size can easily reach the deepest recesses of the lung, the alveoli. As the power changes, so too does the particle black carbon content.

Complementing TEM for particle physical size and nanostructure characterization is X-ray Photoelectron Spectroscopy (XPS) for measuring particle surface chemistry, specifically oxygen functional groups such as phenolic (-OH), carbonyl (-C=O) and carboxylic (-COOH). XPS has also revealed a surprising content of hetero-elements including Ti, Ba, Co, Fe etc. at levels of tenths of atomic percent and higher in the PM exhaust from some aircraft. Particle size, carbon type and elemental composition each bear health implications for exposure to aircraft generated PM at airports and surrounding neighborhoods.

13CB.7

Aircraft Particle Emission from Sustainable Alternative Fuels: Results from Ground Measurements during the NASA/DLR Flight Campaigns ECLIF and ND-MAX. TOBIAS SCHRIPP, Prem Lobo, Joel Corbin, Gregory Smallwood, Ewan Crosbie, Claire Robinson, Michael Shook, Patrick Oßwald, Markus Köhler, *DLR*

There is a large effort underway worldwide to reduce the environmental impacts of aviation through the use of approved alternative fuels blended with conventional Jet A/Jet A-1 (up to 50%). These fuels have been shown to dramatically reduce non-volatile particulate matter (nvPM) emissions. There is also an on-going effort at the International Civil Aviation Organization (ICAO) to develop a correction factors for nvPM emission to account for changes in fuel composition in the development of the regulatory standard.

Within the framework of the combined Emissions and CLimate Impact of alternative Fuels (ECLIF) and ND-MAX campaigns, a series of ground measurements were performed on an Airbus A320-232 "D-ATRA" with V2527 engines at the Ramstein Air Base in Germany. Four different fuels were selected for the campaign due to their expected particle formation potential. Two Jet A reference fuels with low sulfur content and different aromatic contents (19.2 v% and 15.0 v%) were used. The reference fuels were also used to prepare two blends with hydro-processed esters and fatty acids (HEFA) in the range of 49% and 30%. These blends featured 9 v% and 10.1 v% total aromatics, but differed in their chemical composition.

The A320 was operated between idle (23% N1 fan speed) and maximum continuous thrust (82% N1) in discrete power settings that were held stable for approx. 8 min. The particle emission was monitored with particle instruments for size distribution (SMPS, EEPS, OPS), number (CPC), and mass (LII, CAPS, PAX, PSAP, MAAP). In the intermediate thrust settings (60% N1), a reduction in particle emission in the range of 40% can be observed. The difference is negligible at MCT conditions. The decrease in nvPM emissions of the blended fuels relative to the reference fuels was strongly correlated with fuel hydrogen content, which validates the model developed for ICAO.

13CB.8

Variation in Aircraft Engine Aerosol Emissions with Altitude During the NASA ACCESS Campaign. RICHARD MOORE, Kenneth Thornhill, Edward Winstead, Bernadett Weinzierl, Daniel Sauer, Hans Schlager, Claire Robinson, Michael Shook, Luke Ziemba, Bruce Anderson, *NASA*

We present measurements of aerosol emissions indices measured in-situ at various cruise altitudes behind the CFM56-2-C1 engines of the NASA DC-8 aircraft during the 2014 Alternative Fuel Effects on Contrails and Cruise Emissions (ACCESS) project. Aircraft engine emissions can have a disproportionately large climatic impact since they are emitted high in the troposphere and in remote regions with otherwise low aerosol concentrations. This has motivated numerous past ground-based studies focused on quantifying the emissions indices of non-volatile and semi-volatile aerosol species, however, it is unclear the extent to which emissions on the ground translate to emissions at cruise conditions. To better understand these effects, NASA, DLR, and NRC Canada carried out the ACCESS chase plane experiment in 2014. Three different fuel types were investigated including a biofuel blend. Emissions were sampled using a large number of aerosol and gas instruments integrated on HU-25 and Falcon 20 jets that were positioned in the DC-8 exhaust plume at approximately 50-500 m distance behind the engines. It was found that the biojet fuel blend substantially decreases the aerosol number and mass emissions indices, while the gas phase emission indices were similar across fuels. The magnitude of the effects of these fuel-induced changes of aerosol emissions as function of aircraft cruise altitude will be discussed.

13IM.1

Real-time QCM MOUDI for Ambient Aerosol Monitoring. MODI CHEN, Francisco Romay, Robert Anderson, H. Dirk Felton, *TSI Incorporated*

The recently developed Real Time QCM (Quartz Crystal Microbalance) MOUDI (TSI Model 140) was evaluated at the Queens College air sampling station operated by the New York State Department of Environmental Conservation. This evaluation started in December, 2017. Ambient air was sampled from the roof of the site through a PM10 inlet into the instrument at a flow rate of 10 L/min. The temperature inside the sampling site, where the QCM MOUDI was located, was conditioned and maintained at 24 °C. The RH conditioner of the QCM MOUDI had a control set point of 65 %. Therefore, the ambient aerosol sampled by the QCM MOUD was always maintained at 24 °C and 65 % RH, regardless of the outdoor temperature and RH. The performance of the QCM MOUDI was very stable even during the days when the outdoor air temperature was below -10 °C.

The initial data collected during the first two months of measurements was compared with results from a Tapered Element Oscillating Microbalance (TEOM Model 1405 DF) for PM2.5 mass concentrations, and with results from a TSI 3783 water CPC, which measures the total particle number concentration of particles larger than 7 nm. The QCM MOUDI collected particles between 45 nm and 2.5 µm in six size fractions with 15 min time resolution. The total mass collected on all the QCM stages was converted to the PM2.5 mass concentration and was compared with the hourly PM2.5 values measured by the TEOM. The TEOM data showed very abrupt changes from hour to hour. When ambient particle concentration was low, the TEOM sometimes showed negative PM2.5 values for hours. PM2.5 values measured by QCM MOUDI showed less abrupt changes over time, and seemed to report very reasonable PM2.5 values as low as 3 $\mu g/m^3$. The CPC number concentration data was also compared with the QCM MOUDI to check the overall time trends. PM2.5 measured by both QCM MOUDI and TEOM followed similar trends when compared to the total particle concentration reported by the CPC most of the time. The QCM MOUDI data was further compared with daily FRM filter measurements to confirm its accuracy. These preliminary results show that QCM MOUDI has higher time resolution than the TEOM. It is also suitable for measuring the size resolved mass concentration of PM2.5 even at very low particle concentration levels.

13IM.2

Dry Dispersion of Cohesive Powders for Continuous Aerosol Generation in the Sub-micron Size Range. Lekhnath Pokharel, Prashant Parajuli, Li Li, Ewe Jiun Chng, RANGANATHAN GOPALAKRISHNAN, *The University of Memphis*

The dispersion of dry, cohesive micro and nano sized bulk powders has wide applications ranging from medical and environmental science to manufacturing technology. Being able to disperse the dry powder at a stable concentration over periods of time (~hr to several hours) of time is more challenging to achieve, which we attempt to address with a novel dry powder dispersion technology. A portable, cost effective and simple dry powder dispersion device for continuous aerosol production is developed and tested with commercially available powders. Various size of nominal powder sizes ranging from 5 microns, 500 nm, 100 nm and 30 nm (denoting the primary particle size) are considered in this study, to show that the process works for wide range of powder sizes with consistency as well as stability in concentration over time. The study is performed for 5 µm polyamide powder and rutile TiO_2 powders of 500nm, 100nm and 30 nm mean size of primary particles. The device proved to be able to disperse all of these powders, which represent low density material to high density metal oxides, with highly stable and tunable concentration over extended periods. From aerosol measurements to obtain the size distribution of various size particles, it is seen that the the the highly agglomerated powder particles are not easy to de-agglomerate as we go to the lower sized powders because of the stronger inter-particle adhesion forces between nanoparticles compared to microparticles. The SEM images of particles in their native powder state and those collected after the dispersion showed significant difference in the agglomeration of the powder particles, which suggests partial success of the turbulent jet de-agglomeration we have employed for breaking up. We have also tried made improvements based on our findings for to increase the efficiency of dispersion, de-agglomeration and reliability of the device for its commercial use.

13IM.3

Significantly Improving the Operation and Information Yield of Sensor-Type Instrument Densmo by Introduction of a Scanning Mode. PAXTON JUUTI, Antti Rostedt, Jyrki M. Mäkelä, Jorma Keskinen, *Tampere University of Technology, Tampere, Finland*

The use of sensors for measuring aerosols has been steadily increasing in the past years. Sensors are typically simple and affordable in construction, which makes them excellent candidates for measurement networks. On the downside, the sensors might operate on only set parameters, yielding less information than they structurally are able to. To remedy this, parameter scanning is quite commonly used route, which can be seen for example in instrument naming schemes.

In this work, we further develop DENSMO (Juuti et al. 2016), an instrument designed to monitor effective density of aerosol nanoparticles, and introduce a voltage scanning mode to significantly improve its capabilities without doing any structural modifications. The operation of DENSMO is based on the principle of classifying the aerosol first with a zeroth order mobility analyzer and then with a low-pressure impactor. This yields information on both the mobility and aerodynamic behavior of the measured particles, resulting in the values of mobility and aerodynamic median diameters, and consequently the effective density. Without scanning the voltage of the mobility analyzer, the geometric standard deviation of the measured aerosols number concentration needs to be known or estimated based on the source. Thus, one source of uncertainty is completely removed from the operation of DENSMO. In addition, the voltage scanning mode enables DENSMO to give a measure of the fractal dimension of the measured aerosol particles. This is due to the fact that now the effective density is measured as a function of the mobility size.

As DENSMO is designed to be used for monitoring of aerosol nanoparticle synthesis, the performance of the scanning mode is evaluated with spherical and agglomerated nanoparticles made from metal and ceramic particles. For the fractal dimension measurements, in addition to the metal and ceramic particles, also liquid oil droplets are used to ensure the lack of fractality in the particles. These measurements are referenced against scanning mobility particle sizer (SMPS) and electrical low pressure impactor (ELPI), which can be used to measure same particle properties and used to calculate the fractal dimension based on the same particle properties. The results show that the operation of DENSMO is significantly improved by the addition of the voltage scanning mode and, given an aerosol that is inside the working range of DENSMO, the measured values are comparable to the ones retrieved from the reference instrumentation.

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13IM.4

High Resolution Online Measurement of Aerodynamic Diameters Using the Differential Aerodynamic Particle Sizer (DAPS).

DENNIS KIESLER, Thore Rosenberger, Frank Einar Kruis, *University Duisburg-Essen*

Introduction:
The aerodynamic diameter is an important aerosol property to describe, among others, particle deposition as well as particle trajectories in aerosol instruments. The common method to determine this property for nanoaerosols is the measurement with cascade impactors (e.g.: ELPI+, Dekati Ltd; MOUDI-II, TSI Inc.), which have a fast response time but a limited size resolution due to their stage-based design. Instruments with a differential transfer characteristic, where the selected size can be shifted continuously, can obtain a similar high size resolution as the Differential Mobility Analyzer (DMA) for mobility measurements. This comes at the cost of time resolution due to the longer time needed to complete a scan. First instruments offering these for an aerodynamic characterization are the Aerodynamic Aerosol Classifier (AAC, Cambustion Ltd.) (Tavakoli et al., 2014) and the here presented Differential Aerodynamic Particle Sizer (DAPS) (Kiesler and Kruis, 2016, Huber et.al., 2016). Both have the advantage, that the classification is independent of particle charge. The Differential Aerodynamic Particle Sizer is based on a single-orifice aerodynamic lens. The obtainable aerodynamic diameter range is 25 nm to 5 µm. Due to the fast response of the aerodynamic lens, a measurement time of 60s for a full scan with 60 data points is possible.

Setup:
The central part of the DAPS consists of an aerodynamic lens (Liu et al., 1995) with a single orifice. By using sheath gas, a well-defined radial starting position for the particles as well as a particle free central axis are established at the inlet. The orifice focuses a single particle size onto the central axis. These focused particles are then sampled. This gives the DAPS a differential transfer function (Kiesler and Kruis, 2012). The sheath to aerosol ratio a well as the size of the sampler determine the shape of the transfer function. By scanning the pressure in the system, the gas velocity is changed and thus the focused diameter.

This central particle classification part is combined with an unipolar corona charger in front of the inlet and a faraday cup electrometer after the sampling outlet to count the size selected particles. In combination with a pressure sweep, this allows the measurement of an aerodynamic size distribution.

Results:
By using monodisperse particles, it is shown that the DAPS has a differential transfer function. A smaller aerosol to sheath ratio leads to a narrower transfer function. This can be shown in simulation and experiments. A resolution comparable to DMAs is possible. Also the importance of the correct sampling flow to obtain an optimized transfer behavior is shown in simulation and experiments.

Results are presented for two applications. One application is the study of particle behavior at a thin plate orifice at different pressures and flow rates as well as gas compositions. This helps to validate simulations of particle movement with high accelerations and can lead to optimized multi-orifice aerodynamic lens system used in vacuum transfer systems. Another application is the combined measurement of the aerodynamic diameter and the mobility diameter. This combination is a good tool to study agglomerate structure properties (Stein et al, 2013). The high resolution and fast scan time of the DAPS system are well suited for this task. This can be shown by measurements of agglomerates with different fractal dimension.

Acknowledgement:
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13IM.5

Aerosol Charging with a Piezoelectric Plasma Generator. Mario Anton Schriefl, ALEXANDER BERGMANN, Alexander Melischnig, Markus Puff, *Graz University of Technology*

Recently, a new piezoelectric plasma generator, called CeraPlas™, was developed by EPCOS OHG. CeraPlas™ technology provides a platform consisting of the CeraPlas™ piezo ceramic component and a driving stage which allows to build up specific applications for using cold atmospheric plasma. This device allows for high efficient gas ionization at atmospheric pressure and temperature conditions at safe operating conditions. The dimensions, as well as the low power consumption of the device enable its usage for mobile applications. Depending on operating power, surrounding gas flow rate and position downstream of the device, an ion density of up to 2×10^{13} m^{-3} for both, positive and negative polarities, can be achieved. Thus, the device can act as an ion source for aerosol charging. However, in order to use the device for that purpose, some issues related with the operation of the CeraPlas™ — like the emission of nanoparticles and generation of ozone — have to be overcome. In this study we characterize the aerosol charging properties of the device.

Bipolar charging of NaCl particles as a test aerosol was performed by turbulent mixing of particles and ions generated by the CeraPlas™. In order to minimize generation of ozone, and to ensure reproducible working conditions, the CeraPlas™ was operated in N_2 atmosphere. Contamination of nanoparticles emitted by the CeraPlas™ was suppressed by removing them before mixing with the test aerosol, enabled by a specially designed suction channel. This bipolar charging configuration was used as a neutralizer for a differential mobility analyzer and tested against commercially available bipolar aerosol chargers (x-ray source and radioactive source). First promising results show comparable charge distributions and charging efficiencies.

In order to quantify the charging conditions, a multiphysical simulation of the mixing chamber was performed, including fluid dynamics, transport of the ion species and particle trajectories. Assuming the aforementioned ion densities and an ion recombination coefficient of 1.6×10^{12} m^3s^{-1}, we obtained an N_it product about 10^{12} $m^{-3}s$ for this charging configuration. Enhancement of the charging chamber in order to increase the N_it product is ongoing.

A second charging configuration was used which allows for the shift of the charge distribution by use of an electric field in flow direction of the particles. The goal of this method is the adjustment of the charge distribution up to unipolar charging. Artefact formation due to particle emission by the device itself was suppressed by spatially separating the CeraPlas™ from the test aerosols. This configuration resulted in lower charging efficiencies compared to the former method. Nevertheless, first results proof the capability of shifting the charge distribution in either direction, positive and negative. Next steps focus on the optimization of the charging chamber with respect to charging efficiency.

13IM.6

Aerosol Charger Characterization using the Aerodynamic Aerosol Classifier. TYLER J. JOHNSON, Robert Nishida, Martin Irwin, Jonathan Symonds, Jason S. Olfert, Adam M Boies, *University of Cambridge*

Electrostatic classification is a common method used to characterize submicron particles. However these instruments require the aerosol charging characteristics to be known, which directly affects their measurement accuracy (Leppä, Mui, Grantz, & Flagan, 2017). Previous charging characterization studies have largely utilized tandem differential mobility analyzers (DMA) with the aerosol sample passing through the charger of interest between the DMAs. The upstream DMA remains at a constant setpoint, while the downstream DMA resolves each charge-state by stepping through the particle mobility domain of the charged, mobility size-selected aerosol. This experimental setup must be designed and operated to limit the upstream DMA classifying multiple-charged particles and biasing the charging fraction results. Furthermore, due to only a portion of the particles being charged to the desired state, the concentrations measured after being charged and classified twice may be low. This limits the range of particle sizes that can be studied from the same aerosol source, as well as the number of multiple-charged states that can be resolved.

To overcome these challenges, this study used an Aerodynamic Aerosol Classifier (AAC) to characterize different aerosol chargers. The AAC uses a sheath flow at a set rotational speed to select nanoparticles based on their aerodynamic diameter, a property independent of particle charge. This operating principle selects a mono-disperse aerosol source (Tavakoli, Symonds, & Olfert, 2014), making the AAC well-suited for aerosol charger characterization applications.

A BGI Collison nebulizer was used to atomize DOS (bis-2-ethylhexyl sebacate) and produce a poly-dispersed aerosol. The AAC was set at a constant rotational and sheath flow to select a discrete aerodynamic diameter range from the poly-dispersed aerosol. These size-selected particles were then passed through the charger of interest. As a mono-disperse source, each particle charge-state produced a different electrical mobility which was resolved using a DMA stepping through the mobility domain of the AAC classified particles. This methodology was used to measure the negative, neutral, and positive DOS charging fractions at three different particle sizes generated from four different aerosol chargers: a TSI 308701 x-ray neutralizer, two TSI Krypton-85 radioactive neutralizers (one brand new and the other aged for approximately one half-life) and a Cambustion Unipolar Diffusion Aerosol Charger (UDAC). Due to the high transmission efficiency of the AAC relative to the DMA (Johnson, Irwin, Symonds, Olfert, & Boies, 2017), up to 13 charge fractions (6 positive, 6 negative and the neutral) produced from the neutralizers were resolved at each particle size. These results allowed comparison between the chargers as well as against current particle charging theory.

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13IM.7

Differential Diffusion Analyzer. ANSSI ARFFMAN, Paxton Juuti, Juha Harra, Jorma Keskinen, *Tampere University of Technology, Tampere, Finland*

In many areas of aerosol research the interesting particle size range, but at the same time one of the most challenging to study, is from molecules to a few nanometers. For example, atmospheric and anthropogenic nucleation studies investigate particle formation in the sub-3-nanometer size range (Kirkby, 2016; Alanen, 2015). Aerosol measurement instruments that are capable to operate in this size range include high flow rate DMAs, CPCs, and diffusion batteries. A high flow rate DMA connected in series with a low cut-off size CPC offers possibility to measure the particle size distribution down to 2 nm and even below. The major drawback of the DMA based size classification is that particles must be charged prior to the electrical size classification. The charging efficiency of sub-3-nm particles is very low in neutralizers or chargers and depends on many factors as shown by Leppä et al. (2017). This results large uncertainty in the concentration measurement, and furthermore, the charger ions lie in the same size range as the measured particles producing a measurement artefact. The CPC's cut-off size can be varied in order to measure the cumulative size distribution (Vanhanen, 2011) but the detection efficiency is particle material dependent. Diffusion batteries are well-suited instruments to study the sub-10-nm particles and have been developed for in real-time measurement with electrical detection (Fierz, 2002). However, the diffusion stages heavily overlap in size, and thus, the data needs to be treated with advanced inversion methods.

We introduce a new size classifier called a differential diffusion analyzer (DDA; Arffman et al., 2017). This is the first instrument that uses diffusion to differentially size classify aerosol particles, keeping them airborne. The instrument has a flow arrangement similar to a DMA with a sheath and a sample flow, but in the size classification regime there is no electrical field, and particles drift across the sheath flow based on diffusion motion. Therefore, the particles entering the DDA sample outlet have been size selected based on their diffusion coefficient that has an unambiguous and a well-known connection to the mobility particle size via the Stokes-Einstein equation. The main advantage of the DDA is that there is no need for particle charging prior to the DDA, and in addition, it can be used to collect size classified particle samples down to molecular size.

We show theoretically and experimentally that the differential size classification based on the particle diffusion is possible. We studied theoretically a simple DDA geometry where the sample flow is sandwiched between sheath flows, and the sample out flow is drawn from the edges of the two sheath flows. Theoretical investigation results in a simple equation that can be used to roughly estimate the DDA penetrating particle size. With a numerical model we studied how the transmission efficiency function changes with the sheath an sample flow rate ratio and with the total flow rate. It was found that the maximum transmission efficiency of 20% could be achieved while still having a differential transmission function. Experimentally we studied the feasibility of the DDA concept with a cylindrical DMA (TSI model 3071A). With evaporation-condensation generated and monodisperse silver particles, we measured the transmission function of the DMA without electric field. Results verified that with proper sheath and sample flow rates, the transmission function has a differential shape. To further understand the operation, the particle transport inside the DMA with zero electric field was simulated with a CFD model of the DMA.

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13IM.8

Performance Comparison of Corona-based Wire-plate and Needle-mesh Aerosol Chargers. XIAOTONG CHEN, Qiaoling Liu, Jingkun Jiang, Da-Ren Chen, *Tsinghua University*

The performance of a wire-plate aerosol charger and a needle-mesh aerosol charger operated at low DC-corona-discharge current was investigated in this study. Both chargers are designed for miniature electrical particle sizers. The wire-plate charger has an aerosol charging channel established between two metal blocks with a corona discharge chamber embedded in one block. A perforated plate was used to partition the chamber and aerosol charging channel. A Tungsten wire of 50 µm in diameter was installed in the corona chamber for unipolar ion generation when a high voltage was applied on the wire while keeping the perforated plate at the electric ground. Generated ions enter the charging channel via the ion diffusion only. No sheath flow or ion driving voltage was featured in the wire-plate charger. An aerosol flow was injected into the aerosol charging channel via the inlet tube and exited from the outlet tube. The needle-mesh aerosol charger was modified from the mini-charger (Qi et al., 2008) by replacing the perforated dome-shaped end of the corona-discharge tube with a flat-meshed end. A tungsten needle was positioned at the center of corona tube for ion generation. An ion-driving voltage of 30 V was applied between the corona tube and charge case to drive ions into the aerosol charging zone established between the corona tube and charger case. Both chargers were operated at their optimal operation conditions except that the corona current was kept at 0.3 µA for the low energy consumption while achieving high charging efficiency.

Both intrinsic and extrinsic charging efficiencies of particles with different mobility diameters achieved by the chargers were measured. The wire-plate charger has lower intrinsic charging efficiencies than the needle-mesh charger. For the wire-plate charger, the extrinsic charging efficiencies at the aerosol flow rate of 0.3 lpm are slightly higher than that at the flow rate of 0.6 lpm. The extrinsic charging efficiency of the wire-plate charger remains approximately 80% for particles larger than 40 nm. For the needle-mesh charger, its extrinsic charging efficiency at the 0.6 lpm aerosol flow rate was higher than that at the flow rate of 0.3 lpm for particles greater than 60 nm. The trend was reversed for particles less than 60 nm. Large particles carry more electrical charges and lose more due to the presence of weak electrical field and the increased residence time in the charging zone at the 0.3 lpm aerosol flow rate. The extrinsic charge distributions of particles with mobility sizes less than 300 nm were also characterized. It is found that multiple charge effect was observed for particles with the sizes larger than 20 nm in the wire-plate charger, and the wire-plate charger attached fewer charges on particles than the needle-mesh one.

The performance of both chargers was also evaluated via the birth-and-death charging model with the ion-particle combination coefficients estimated using the Fuchs limiting sphere theory. Reasonable agreement was achieved between the calculated and measured charging efficiencies. The discrepancy between the experimental and calculated charge distributions could be attributed to the loss of charged particles and the spatial non-uniformity of ions in the charging zone. A Gaussian distribution function was further proposed to fit the measured particle charge distributions.

13MG.1

Air Quality in the Megacity of Beijing: From Sources to Control. MIN HU, Dongjie Shang, Yao Xiao, Jing Zheng, Song Guo, Zhijun Wu, Keding Lu, Limin Zeng, Sihua Lu, Shaodong Xie, Yuanhang Zhang, *Peking University, Beijing, China*

Severe regional haze problem in the megacity of Beijing and surrounding areas has attracted much attention in recent years. It has the characteristics of rapid accumulation of PM2.5 pollution within 5 to 7 days duration, covering large areas. The presentation will give an overview on emissions reduction policies developed and implemented by the Chinese government. The Action Plan on Prevention and Control of Air Pollution (so called “Ten Major Measures” for air pollution) was conducted in 2013-2017. As the results the number of days of heavy air pollution (mainly occurred in winter) in Beijing was 58, 47, 46, 39, 23 days in 2013-2017, respectively, showing a decreasing feature year by year. The days of heavy pollution decreased by 35 days within five years, and the incidence of heavy pollution decreased significantly. PM2.5 also decreased significantly from 89.5 µg/m3 in 2013 to 58 µg/m3 in 2017. The spatial distribution of the whole Beijing area was still high in the south and low in the north, but the gap between the north and the south decreased.

The interplay between source emissions, atmospheric chemical mechanisms, meteorological conditions and aerosol thermodynamics is non-linear and quite complex. It is a great challenge to implement effective mitigation strategies. In order to obtain scientific understanding of haze pollution, we conducted intensive field campaigns, chamber simulation and modeling studies in Beijing and surrounding areas for years. Our results revealed that haze formation includes two processes: “seeds” production (efficient nucleation, primary emission) and rapid particle growth. During the pollution episodes secondary compounds (SNA, SOA) dominated in particle mass concentrations. The presentation will focus on source apportionments of PM2.5 and the mechanisms of chemical process during the haze formation in the wintertime of Beijing.

13MG.2

How Much Emission Reduction is Needed to Meet Ambient PM2.5 Standards in the Cities of Sichuan Basin? XUE QIAO, Wenye Deng, Hao Guo, Ya Tang, Jianlin Hu, Qi Ying, Hongliang Zhang, *Sichuan University; Louisiana State University*

Sichuan Basin (SCB) in southwestern China is one of the three regions that are most affected by haze in the country. During 2013 to 2016, annual average PM2.5 concentrations were 63-96 and 54-70 μg m-3 in Chengdu and Chongqing, respectively, which are the economic, education, and transportation hubs in southwestern China. The total population of 110 million in the 18 cities in the 221,000 km2 SCB are in severe risks. Therefore, it is important to investigate how to mitigate PM pollution. PM pollution in the SCB is mainly associated with the high anthropogenic emissions within the basin and the basin landform, which favors air pollutants accumulated and transported across cities within the basin. This study uses a source-oriented version of the Community Multi-scale Air Quality (CMAQ) model to quantify (1) contributions of different geographical regions to PM2.5 concentrations in the SCB and (2) PM2.5 reduction in these cities under different emission scenarios. As PM2.5 concentrations are highest in winter and lowest in summer, the simulations were performed only for January and August, 2015. The predictions of meteorology (including ambient air temperature, wind speed, wind direction, and relatively humidity) and PM2.5 concentrations were generally in agreement with the observations, giving the confidence in model performance. The results confirmed that the anthropogenic emissions within the basin were the major sources of PM2.5, and inter-city transport of air pollutant within the basin had significant contributions. These suggest the importance of reducing air pollutant emission within the basin in order to improve air quality for the 18 cities. Application of the state-of-art of emission reduction technologies in industries, domestic activities, and power plants can greatly reduce PM2.5 concentrations in the basin, but PM2.5 pollution would be still a problem in some areas, indicating there is a need to adjust the economic and energy structures in the SCB. The environmental capacities of air pollutant emissions for the two largest cities, Chengdu and Chongqing, were also estimated.

13MG.3

Improved Air Pollution Control Incentive Measures and Regulations in the South Coast Air Basin with an Holistic Energy and Emissions Model. SCOTT A. EPSTEIN, Marc Carreras-Sospedra, Xinqiu Zhang, Sang-Mi Lee, *South Coast Air Quality Management District*

The South Coast Air Basin of California is a region encompassing the greater Los Angeles area with approximately 16 million residents and 11 million vehicles. While air quality has markedly improved in past decades, significant challenges remain. Topographical constraints on pollutant transport, favorable meteorology, and a strong reliance on fossil fuel combustion in the transportation and industrial sectors has led to elevated ozone and $PM_{2.5}$ concentrations that exceed federal ambient air quality standards. The 2016 Air Quality Management Plan—a regional blueprint for achieving air quality standards and healthful air—relies on a comprehensive framework of regulations and incentive programs to achieve air quality goals.

It is critical to allocate incentive funds and design regulations to implement projects providing the largest pollutant reduction per dollar spent, yet comparing the cost effectiveness of technology retrofits in the residential and commercial sector involving different fuel types has traditionally been difficult. In order to holistically identify the most cost-effective measures, we developed the Net Emission Analysis Tool (NEAT). NEAT is a comprehensive model designed to determine the resulting region-wide NOx and greenhouse gas emission reductions expected in the retrofit of residential and commercial technologies including appliances, battery storage, and distributed solar energy generation. NEAT models the change in natural gas and electric utility bill costs, appliance costs, point-of-use emissions, and electricity generation emissions resulting in a user-defined retrofit scenario. We will employ NEAT to help identify incentive measures and develop regulations that are highly cost-effective in terms of NOx and greenhouse gas emission reductions. With the results from NEAT, we will use the Community Multiscale Air Quality Modeling System (CMAQ) to determine the resulting impacts on ozone and $PM_{2.5}$ concentrations. An holistic evaluation of air pollution control measures will maximize ozone and $PM_{2.5}$ reductions throughout the South Coast Air Basin.

13MG.4

Quantifying Feedbacks between Pollution, Radiation and Boundary Layer Dynamics in Beijing. JESSICA SLATER, Gordon McFiggans, Hugh Coe, Sami Romakkaniemi, Juha Tonttila, Paul Connolly, David Topping, Pingqing Fu, Yele Sun, Simone Kotthaus, Zhijun Wu, *University of Manchester*

Atmospheric aerosol concentrations globally have increased due to anthropogenic activities, such as industry, heating, transport and cooking. Increased aerosol concentrations can result in severe pollution events, particularly in urban mega-cities. The severity of pollution events is often characterised by concentrations of PM2.5 (particulate matter with a diameter of 2.5 µm or less), which are believed to have an impact on human health, through their ability to enter into the lungs, alveoli and blood stream. Beijing, is a megacity which is well-known for poor air quality, often subjected to heavy pollution events termed 'haze'. A major UK-China field campaign took place over 2016/2017 with the aim of furthering understanding of the pollution processes in Beijing and potential impacts on human health. An aerosol-radiation-meteorology feedback loop is likely to be a strong factor in the formation and longevity of these heavy pollution episodes.

Large Eddy Simulations (LES) are a type of small scale model which can explicitly model turbulence, specifically large eddies while ignoring very small scale processes. A novel LES model with an additional aerosol module, UCLALES-SALSA, will be used to assess characteristics, growth and lifetime of heavy pollution episodes. Particularly with the aim of quantifying interactions between aerosols, radiation and meteorological variables, such as boundary layer height. Measurements taken during the campaign in Beijing, including aerosol and tower measurements are used to initialise a vertical profile for the model as well as for result comparison.

13MG.5

Dirty Jets: Observations of Ultrafine Particle Plumes from Landing Aircraft at Boston Logan Airport and a Data Science Approach to Identify the Culprits. Scott Hersey, Allen Downey, Caz Nichols, EBEN CROSS, *Franklin W. Olin College of Engineering*

We present data collected at a community partner's home on the approach path to runway 27 at Boston Logan Airport during 3 weeks of sampling during 2017 and 2018. During periods of active landing on runway 27, aircraft passed the sampling site at a distance of 110 m and an average altitude of 75 m, with intervals of 30-300 s. During runway 27 use, plumes of particles with size mode between 10 and 30 nm were observed within 40-60 s of aircraft fly-by, and reached concentrations of 100,000 to 500,000 cm^{-3} before exponential concentration decay as plumes dispersed. Plume concentration varied substantially between aircraft. A tool was built in python to construct a database of aircraft landing and take-off events at the airport from publicly available FAA data, extracting aircraft type and carrier as well as position and altitude. Thrust behavior when passing the study site was inferred from the derivative of descent trajectories, thereby allowing for an investigation into the most important factors determining plume strength from descending aircraft – namely aircraft/engine type and thrust behavior. We will present gas-and particle-phase measurements, details of our participatory, community-driven approach, and a description of the python tool and its development.

13MG.6

Effects of Diesel Truck Regulations on Environmental Justice in a Major Freight Corridor in California. REGAN PATTERSON, Robert Harley, *University of California, Berkeley*

Freight transportation is a major source of diesel pollution in California. Communities in freight corridors are disproportionately burdened by exposure to diesel truck exhaust and related health impacts. Residents in these corridors are predominately nonwhite and low-income. To reduce diesel truck emissions, California regulations require an accelerated adoption of control technologies. The phase-in of diesel particle filters (DPFs) began in 2010, and all heavy-duty trucks were required to be equipped with DPFs by January 1, 2014. While these regulations have resulted in emission reductions, the impact on exposure disparities has not been analyzed.

In this study, we model the effect of control technologies on equity. This study focuses on the major freight corridor in East Oakland that serves the Port of Oakland, Oakland International Airport, and industrial facilities. Heavy-duty trucks are prohibited on the highway (I-580) located in the Oakland Hills and must travel on the highway (I-880) in the Flatlands, which are predominately nonwhite, low-income communities. We estimate nitrogen oxides (NO_x) and black carbon (BC) emissions on both highways before (2009) and after (2015) the adoption of control technologies. We use the RLINE dispersion model to simulate the effect on concentrations at Census block level in two neighborhoods downwind of the I-880 and I-580. We estimate population intake and changes in indicators of environmental justice and equality to quantify the impact of diesel truck regulations on health benefits and exposure disparities between communities.

13MG.7

Air Pollution in Latin American Cities. Hector Jorquera, LUPITA MONTOYA, Nestor Rojas, *University of Colorado Boulder*

The World Health Organization (WHO) estimates that in 2014, 92% of the world population was living in places where the WHO air quality guidelines levels were not met. According to WHO's Global Urban Ambient Air Pollution Database, there are 122 cities in 16 Latin American countries that routinely report ambient concentrations of PM10 and PM2.5. The air quality at some of the largest cities in Latin America has been improving in recent years; however, the ambient air quality standards are still not attained in many of them. For countries that only report air quality for their capital cities, their pollution levels are often above the respective national ambient air quality standards. Most of the data compiled by WHO are estimates based on PM10 measurements because ambient PM2.5 is less frequently measured throughout the region. In addition, there is less information about air quality for mid-size cities, in countries like Brazil, Chile, Ecuador and Mexico, where the most polluted city is not the country's capital.

Source apportionment studies have been conducted in several Latin American cities that don't meet the WHO's guideline of 10 ug/m3, as long-term averages. In general, coastal cities like Rio de Janeiro and Recife in Brazil have better air quality than continental cities in valleys surrounded by mountains like Córdoba in Argentina, México City in Mexico, Medellin in Colombia and Santiago in Chile. Ambient PM2.5 has decreased in Rio de Janeiro, Sao Paulo and Santiago, with traffic sources increasing and industrial sources decreasing in relative contributions. These trends likely reflect increases in motor vehicles and more regulations imposed on industry.

There is scant information about the state of indoor air quality (IAQ) in Latin America. The emphasis so far has been on ambient air quality and advancing ambient air regulations in the region; however, there have been a few IAQ studies conducted in urban settings. Indoor air quality regulations in Latin America have revolved primarily around enacting smoke-free policies after the adoption of the WHO Framework Convention on Tobacco Control (FCTC) in 2005. The FCTC provided the needed mechanisms to enable national and subnational legislations to effectively protect people from second hand smoke. Since then, several Latin American countries have enacted smoke-free policies in public places. Some local smoke-free policies have been enacted in places like Mexico City. All these initiatives have been encountered by strong opposition from the tobacco industry, which has often turned to litigation to stop them. In general, the preponderance of the burden of indoor air pollution is faced by the poorest sectors in Latin American countries, often the rural and urban poor. The associated health effects due to indoor air pollution exposures in these communities have received limited attention and much of what we know is deduced from studies conducted in developed countries at much lower pollution levels. In this work, case studies from several Latin American countries are discussed in terms of air quality, environmental justice, urban governance and citizen participation in decision-making processes, sustainable urban transport options and gender issues.

13MG.8

Seasonality of Air Pollution in Bogota: From Regional Biomass Burning Transport to Local Sources. RICARDO MORALES BETANCOURT, Luis Carlos Belalcazar, Juan Felipe Mendez, Maria Paula Perez-Peña, Yadert Contreras Barbosa, Juan Pablo Ayala, *Universidad de los Andes*

In this research we determined the salient aspects controlling the seasonality of air pollution levels in the city of Bogota. Bogota is a large metropolitan area located in the northern South American Andes. With a population of nearly eight million inhabitants, Bogotá has experienced a rapid growth in motorization rates and the air pollution levels in the city very often exceed WHO limits. Many studies have focused on the large impact of local mobile and industrial sources on local air quality. However, there is a lack of understanding of the role that meteorological variables and long-range transport of pollutants can have in the seasonal variations of air pollution levels in the city. The precipitation and hence biomass burning seasons in northern South America are markedly different to those of Amazonia. Despite the fires in northern South America are not a significant contributor to global inventories, they can potentially impact regional air pollution levels. In this work we quantify the contribution of meteorological conditions and regional transport of biomass burning plumes to the seasonality of particulate matter pollution in the city. The climatology of variables impacting atmospheric stability in the northern South American Andes are determined both through a decade-long record of radiosonde data, as well as reanalysis data. The seasonal cycle of particulate pollution in the city is shown to be only partially explained by the climatology of atmospheric stability indices. The potential of biomass burning plumes transported to the city during the dry season is explored here as a candidate variable to explain the remaining unexplained seasonal variability in PM pollution. We used 10 years of MODIS Active Fire Data and HYSPLIT calculated back-trajectories. The number of fires that could impact the air quality in the city is determined by considering only those hot-spots located within a spatial buffer of the HYSPLIT simulated back-trajectory location for air masses reaching the city. In this way only, those fires that are potentially causally related to air pollution levels are accounted for. Two meteorological datasets were used to run the HYSPLIT back-trajectory model finding similar results. A strong correlation between the number of fires detected with this method and PM10 and PM2.5 levels is observed. Finally, we performed simulations with the WRF-Chem chemical transport model coupled to meteorology, to model the long-range transport of biomass burning pollutants during the dry and wet seasons. Our study suggests that a significant portion of the seasonal variations in PM pollution levels for the city of Bogota can be explained by seasonal changes in atmospheric stability and seasonal regional transport of biomass burning plumes. The contribution of local sources is isolated in the simulation performing sensitivity analysis to mobile and industrial local sources from a local emission inventory.

13SA.1

Source Apportionment of Brown Carbon Absorption by Coupling Ultraviolet-Visible Spectroscopy with Aerosol Mass Spectrometry. VAIOS MOSCHOS, Nivedita Kumar, Kaspar Rudolf Dällenbach, Urs Baltensperger, Andre S.H. Prévôt, Imad El Haddad, *Paul Scherrer Institute / ETH Zurich*

The optical properties and sources of atmospheric aerosols are of prime importance in the context of a changing climate.[1] Primary and secondary organic aerosol (OA) emissions introduce light-absorbing compounds (brown carbon, BrC) in the atmosphere that affect tropospheric chemistry and might exert, along with soot carbon, a significant direct radiative forcing on the climate system.[2] This effect has been largely acknowledged[3] but remains uncertain, since either most climate models have been ignoring the contribution of BrC to absorption or the associated mixed emission sources[4] and atmospheric lifetime[5] are not accounted for.

In this work, we propose positive matrix factorization (PMF) as a framework to apportion the contributions of individual primary and secondary OA source components of BrC absorption, by combining long-term aerosol mass spectrometry (AMS) data with concurrent ultraviolet-visible spectroscopy measurements. The former feature time-dependent factor contributions to OA mass[4] and the latter consist of wavelength-dependent absorption coefficients, determined using real-world mixed-source samples.

Using this approach for a full-year case study, we estimate for the first time the mass absorption efficiency (MAE) of major light-absorbing water-soluble OA components in the atmosphere. We show that secondary biogenic emissions, largely consisting of low molecular weight monoterpene oxidation products, contribute negligibly to absorption despite dominating the mass concentration in summer. In contrast, the MAE of strongly absorbing BrC from primary and aged wood burning emissions can be constrained within a confined range. For the primary emissions, this range is consistent with previous laboratory tests of open and residential burning of biomass or other fuels and near-source ambient samples, but lower than non-conventional BrC types (e.g., funeral pyres and humic-like substances). The MAE of the aged emissions follows that of common anthropogenic precursor (benzene, naphthalene, toluene) secondary OA formed under high NO_x conditions. We note the reduced MAE of aged vs primary wood burning emissions at most wavelengths, in agreement with recent laboratory experiments and a post-biomass-burning event observation.

The MAE constrained here can be used to predict the impact of the identified BrC sources on climate, through Mie calculations and radiative transfer modeling. This novel platform may be applied to other datasets, including environments that are heavily polluted or largely represented by other sources (e.g. coal combustion in China). The approach may also be suited for online datasets, acquired using aerosol mass spectrometry and various online optical measurement techniques. The sensitivity of the PMF model results to the applied mass spectrometric analysis has to be assessed in similar future studies.

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13SA.2

Wintertime Study of Ambient Aerosols (PM1 and PM2.5): Insights to Source Characterization and Atmospheric Transformation. GYANESH KUMAR SINGH, Prashant Rajput, Pradhi Rajeev, Dharmendra Kumar Singh, Amit Kumar Singh, Debajyoti Paul, Tarun Gupta, *Indian Institute of Technology Kanpur*

Indo-Gangetic plain (IGP) is heavily polluted especially during winter-time due to its topography, meteorological conditions and elevated particulate (PM) emissions. Various studies have been conducted to understand the sources as well as different processes undergoing in the atmosphere over this region. For a better understanding of the contribution of various sources to aerosols, stable isotope ratios have been assessed in this study. Ambient aerosols (PM_1 and $PM_{2.5}$) collected during wintertime from Kanpur (central part of IGP) were studied for their chemical composition such as organic carbon (OC), elemental carbon (EC), water-soluble organic carbon (WSOC), water-soluble inorganic species (WSIS) and stable carbon isotope composition ($\delta^{13}C$). During the study period, predominant origin from north-west direction was seen in the air-mass back trajectories arriving at the receptor site. PM mass along with higher total carbonaceous aerosols (TCA) concentrations can be attributed to the impact of massive emissions from anthropogenic sources (vehicular exhaust, industrial emissions, and biomass burning) and meteorological conditions like low wind speed and low mixing height. The contribution from OC was nearly 22% and 15% and EC was nearly 2% and 0.14% of ambient $PM_{2.5}$ and PM_1 mass respectively. There is a significant increase in the concentration of ions like NH_4^+, NO_3^-, and SO_4^{2-} during this time period due to stagnant air condition and various fog/haze events. Variability in aerosol mixing comprising of primary and secondary emission products can be deduced from observed significant variability in OC/EC ratio and WSOC/OC ratio in ambient samples. $\delta^{13}C$ of TC in ambient aerosols found were quite comparable in both $PM_{2.5}$ and PM_1 in this study. $\delta^{13}C$ of samples from some possible sources (coal, gasoline, diesel, and bio-diesel) were analyzed to ascertain their different characteristics. Also, the possible contribution from several sources can be inferred from large scatter between $\delta^{13}C$ and TC content. Variable $\delta^{13}C$ in short and long-range transported aerosols suggests the plausibility of mixing of variable sources of carbon resulting in the observed variability of $\delta^{13}C$.

13SA.3

Carbonaceous Organic Aerosol Composition and Sources in the Baltic. ATHANASIA VLACHOU, A. Tobler, Houssni Lamkaddam, Carlo Bozzetti, Kaspar Rudolf Dällenbach, Gary Salazar, Soenke Szidat, Urs Baltensperger, Imad El Haddad, Andre S.H. Prévôt, *Paul Scherrer Institute*

Organic aerosol (OA) is linked to adverse climate and health effects. It is often separated in primary OA (POA) which is directly emitted as particles and in secondary OA (SOA) which is formed in the atmosphere via oxidation of volatile organic compounds. A robust method to study the composition and identify the sources of both POA and SOA is the "offline AMS" technique, which combines aqueous filter extracts measurements with the Aerodyne aerosol mass spectrometer (AMS) and statistical analysis of the resulting organic spectra with positive matrix factorisation. The use of filter samples allows for fast analysis of long term measurements, spatial broadening of the OA monitoring, as well as independence in aerosol size cut-off. In parallel, the radiocarbon analysis of ambient filter samples provides an unequivocal separation between fossil and non-fossil sources, by determining the 14C content of the total carbon. The combination of these two techniques significantly boosts our understanding of the POA and SOA sources.

Despite the few reports on source apportionment and chemical composition of OA in the Baltic region, the coupling of the two techniques has never been applied on filters from this region before. Therefore, the fossil and non-fossil sources of POA and SOA and their seasonal variation still remain unknown. Here we show the combined offline AMS and radiocarbon analysis of OA (particulate matter <10µm), for one year (2013-2014), at three sites in Estonia and three in Lithuania that represent both rural and urban environments. Biomass burning during winter and primary biological OA during late spring and summer are the two most important primary organic aerosols. However, the SOA plays a more crucial role during these two periods with connections to anthropogenic, non-fossil, emissions in winter and biogenic in summer. This is also in agreement with other studies of OA in several European sites where the non-fossil SOA is the main driver in mass.

13SA.4

Sulfuric Acid and Nanocluster Aerosol Measured in an Urban Street Canyon of Helsinki, Finland. MISKA OLIN, Riina Hietikko, Minna Aurela, Heino Kuuluvainen, Niina Kuittinen, Mia Isotalo, Hilkka Timonen, Jarkko Niemi, Topi Rönkkö, Miikka Dal Maso, *Tampere University of Technology*

New particle formation (NPF) in urban air is important for human health and various atmospheric processes. Gaseous sulfuric acid (GSA) is often shown to be associated with NPF. However, its connection to 1-3 nm sized particles, called nanocluster aerosol (NCA), has not been widely studied in traffic-related environment. NCA concentration is an important quantity in terms of NPF because it is connected to the initial steps of the particle growth process. However, according to recent findings, NCA can be a direct result of road traffic emissions in urban areas rather than being connected to the atmospheric nucleation process often induced by photochemistry. While GSA and sub-3 nm particles have been concurrently measured in continental pristine and background areas, we present the first simultaneous measurement of GSA and NCA at urban roadside areas. This enables better understanding of the formation process of NCA and its connections to, e.g., traffic density.

The GSA concentration was measured in a street canyon (traffic density: 28 000 vehicles/weekday, 10% heavy duty vehicles) using a nitrate-based chemical-ionization atmospheric-pressure-interface time-of-flight mass spectrometer (CI-APi-TOF) in May 2017. The measurement was performed in a Supersite air quality monitoring station located near the city center of Helsinki, Finland. The continuous time series of GSA concentration provides information on the diurnal variation of the GSA concentration, and the influence of solar radiation, traffic density, and other environmental variables on the GSA concentration. The NCA concentration was measured simultaneously at the same location using an Airmodus Particle Size Magnifier (PSM) and a TSI Condensation Particle Counter (CPC). In addition, also other aerosol and gas measurement devices were used in the campaign.

The highest GSA concentrations were observed during the rush hours but increased concentrations were also observed after midnight, when the traffic density was the lowest. The diurnal variation of the GSA concentration had a correlation with the diurnal variation of the NCA concentration.

13SA.5

Identification of the Chemically Distinct Groups of Atlantic Aerosol Particles from 53°N to 53°S. SHAN HUANG, Laurent Poulain, Wolfram Birmili, Zhijun Wu, Hartmut Herrmann, Alfred Wiedensohler, *Jinan University*

The marine aerosol plays an important role in global climate regulation and marine biogenic system. However, aerosol particles in the marine boundary layer (MBL) are seldom from exclusively marine origins. Complex sources and atmospheric processes determine the chemical and physical properties of aerosol particles. In this study, chemically distinct groups are identified by k-means clustering, in an exploratory way, on chemical composition (provided by a High Resolution Time of Flight Aerosol Mass Spectrometer, HR-ToF-AMS) and particle number concentration (PNC) of MBL aerosol particles, and linked to the air mass origins. The analysis is based on physical and chemical measurements performed on board the German research vessel Polarstern during 4 research cruises over the Atlantic Ocean in 2011 and 2012, covering spatial range from 53°S to 53°N in two seasons (spring and autumn). In total 12 variables were used for clustering, including PNC of aerosol particles and 11 chemical components (ammonium, nitrate, chloride and BC directly provided by instruments, plus 5 organic components and 2 sulfate components with identified sources given by source apportionment models). With this algorithm, a total of 4 clusters was identified based on the distinct chemical composition corresponding to 2 marine types and 2 continental types. Moreover, when compared to air mass back trajectories, each cluster can be attributed to a specific air mass type and/or influenced by location. Specifically, the marine 1 cluster was characterized by dominating contribution of dimethyl sulphide (DMS) oxidation products, coincidently with air masses from the ocean. The marine 2 cluster containing significant nitrogen products, which could be attributed to biogenic amines sources, was found mainly in autumn (especially over the Southern Atlantic) within marine air masses. The continental cluster appeared only in the Northern Hemisphere, in most case associated with air masses from the Europe. The combustion cluster occupied a wide area between 15°S and 15°N in autumn (November), influenced by the seasonal continental outflow (e.g. biomass burning). The resulting clusters are repeatable in the same season along the similar ship tracks, which makes the method useful for modelization on predicting physicochemical properties of MBL aerosol.

13SA.6

Source Apportionment of Organic Particulate Matter at the Phillips 66 Research Center in Bartlesville, Oklahoma.

SHAOKAI GAO, *Phillips 66 Research Center*

An understanding of emission sources of primary particulate matter (PM) and chemical reaction pathways leading to formation of secondary organic aerosol (SOA) is critical to implementing effective PM control strategies. Organic PM is the least understood component of atmospheric PM. During the last several decades, use of online aerosol mass spectrometry coupled with positive matrix factorization (PMF) analysis has advanced the understanding of the origin and transformation of organic PM.

In the present study, an eight-week field campaign was conducted at the Phillips 66 Research Center in Bartlesville, OK to measure non-refractory, sub-micrometer organic PM, identify emission sources, and describe potential chemical reaction pathways of SOA formation. An aerosol chemical speciation monitor (ACSM) was used to measure organic PM. The PMF method was used for the source apportionment, which identified seven emission factors of organic PM. Gasoline vehicle exhaust, diesel vehicle exhaust, biomass burning, and industrial stationary source emissions were identified as primary emission factors. Low-volatile oxidized organic aerosols (LV-OOA), semi-volatile oxidized organic aerosols (SV-OOA), and oxidized organic aerosols from biomass burning (OOA-BB) were identified as secondary emission factors. The study found that SOA comprised 63% of measured organic aerosol mass loading. SOA formation during the daytime was mainly driven by photochemical reactions of aromatics and alkanes, which was highly dependent on the UV intensity. Of the seven identified emission factors, the biomass burning related organic aerosols and LV-OOA, (also known as long-range transported organic aerosols), which are considered as “uncontrollable” emissions, comprised more than 60% of organic aerosol mass loading. This study has helped in advancing the understanding of PM emissions and transformation processes in northeast Oklahoma due to the lack of data in the literature from this area.

13SA.7

Multi-Year Source Apportionment of Highly-Time Resolved Carbonaceous Aerosol in the Region of Paris, France.

YUNJIANG ZHANG, Olivier Favez, Francesco Canonaco, Jean-Eudes Petit, Tanguy Amodeo, Francois Truong, Jean Sciare, Andre S.H. Prévôt, Valerie Gros, Alexandre Albinet, *INERIS*

Carbonaceous particulate matter accounts for a large fraction of fine atmospheric aerosol particles and plays a significant role on air quality and climate forcing. Although various primary sources and secondary transformation processes have already been identified and quantified worldwide, its characterization over long-term time periods remains poorly documented. We report here the first source apportionment of carbonaceous aerosols for a 5$^+$-year period from in situ on-line measurements at a suburban background site (SIRTA) located in the Paris region (France). Submicron non-refractory aerosols were measured using an aerosol chemical speciation monitor (ACSM) with a 30-min time resolution, while equivalent mass concentration of BC was measured by a seven-wavelength aethalometer with 1 min frequency. The relative source contributions of wood burning and traffic emissions to black carbon were estimated using the ‘aethalometer model’. Positive matrix factorization, based on ME-2 engine, was applied to apportion the organic aerosol (OA) sources using the advanced Source Finder toolkit (SoFi Pro), specifically designed to robustly identify the expected factors even over multi-year time scales. Results obtained with SoFi Pro were then compared to the standard SoFi outputs, corresponding to 12 successive ME-2 computations for the 2014-2017 period. Converging results nicely illustrated seasonal, weekly, and diurnal cycles of the various primary and secondary carbonaceous aerosol fractions, and offer a unique immersion into the seasonal characteristics of secondary OA (SOA) in Paris. Primary carbonaceous showed higher concentrations in winter due to enhanced wood burning emissions during the heating season. SOA dominated the total carbonaceous aerosol loading all around the year as a result of regional transport and local physicochemical formation processes. Less- and more-oxidized SOA fractions have been highlighted for the entire studied period. Finally, the impact of aqueous (heterogeneous) and photochemical processes on the SOA formation was also addressed.

13SA.8

Chemical Characterization of Secondary Organic Aerosol (SOA) in a Transitional Season of Biogenic VOC Emission.

YUNLE CHEN, Theodora Nah, David Tanner, Masayuki Takeuchi, Hongyu Guo, Amy P. Sullivan, Lu Xu, Rodney J. Weber, Greg Huey, Nga Lee Ng, *Georgia Institute of Technology*

The formation and evolution of SOA was investigated at Yorkville, a rural site 55km NW of Atlanta, in late summer (mid-August ~ mid-October, 2016), a period when the biogenic volatile organic compounds (VOC) emissions were gradually decreasing. This is a rural site in the Southeastern Aerosol Characterization (SEARCH) network, situated in a mixed forest–agricultural area and is characterized by intense agricultural emissions. A High-Resolution Time-of-Flight Mass Spectrometer (HR-ToF-AMS) was deployed to characterize non-refractory submicron particles. Co-located instruments (CIMS, FIGAERO-CIMS, GC-MS, PILS-IC, etc.) were used to comprehensively characterize both gas- and particle-phase composition.

Unconstrained Positive Matrix Factorization (PMF) analysis and Multilinear Engine (ME-2) analysis with constrained profiles are applied to identify and quantify OA sources. Prior measurements at the same site suggest that biogenic SOA is a predominant source of total OA at the Yorkville site, where contribution from isoprene-derived OA (Isoprene-OA) to total OA is 36% in summer (July), but nearly zero in winter (December). In this study, the continuously decreasing isoprene emission throughout the measurement period poses a challenge to resolving isoprene-derived OA using PMF. With constrained Isoprene-OA profile (from Centreville measurements during 2013 summer, resolved by PMF), ME-2 analysis successfully resolved four factors, including Isoprene-OA, less-oxidized oxygenated OA (LO-OOA), more-oxidized oxygenated OA (MO-OOA), and a possible sesquiterpene-derived OA (Sesquiterpene-OA).

With isoprene emission decreasing and NO concentration relatively constant, we observed a clear shift of isoprene oxidation pathways from “low-NO_x” chemistry to “high-NO_x” chemistry, as NO / isoprene ratio increased. Our measurements of gas-phase organic acids (e.g. formic acid) show good correlation with isoprene-OA, suggesting isoprene aerosol formation processes are possibly an important source for atmospheric organic acids, which is consistent with recent studies that isoprene photooxidation is an important contributor to atmospheric organic acid budget. Meanwhile, we observed a good correlation between MO-OOA factor with the sum of particle-phase organic acids (C_2 – C_5 acids, Pearson’s $R^2 = 0.83$), suggesting that the ubiquitous MO-OOA factor could be composed of particulate organic acids. The LO-OOA factor and Sesquiterpene-OA factor show correlation with particulate C_{10} and C_{15} organic nitrates, indicating possible aerosol sources from nitrate radical chemistry and/or photooxidation in the presence of NO_x.

13TO.1

Effect of Combustion Particle Size on Pathologically Important Responses in Lung Cells. KAMALJEET KAUR, Raziye Mohammadpour, Isabel C. Jaramillo, Robert Paine, Chris Reilly, Hamid Ghandehari, Kerry Kelly, *University of Utah*

Although combustion-derived particulate matter(cdPM) is a significant contributor to fine and ultrafine PM levels, our understanding of its health effects is complicated by cdPM's complex nature: a dynamic mixture of particles and condensed material with different sizes, shapes, and chemical compositions that is generated from a range of sources. Furthermore, several confounding factors make comparing results from various studies of PM's adverse effects difficult including, for cdPM, fuel composition, the age of the combustion device, combustion conditions, lubricants, and sampling methods. For example, experimental and epidemiological studies about the effect of various PM size fractions (PM_{10}, $PM_{2.5}$, and PM_1) provide somewhat conflicting results. As particle size diameter decreases, its relative surface area increases, which in turn increases the bioavailability of atoms or molecules and may lead to increased pro-inflammatory effects. This study focuses on directly testing the effect of cdPM size on biological responses in lung cells.
cdPM with consistent properties is generated from a premixed flat-flame burner combusting a jet-fuel surrogate at an equivalence ratio of 2.5. A nitrogen shroud and a glass housing minimize atmospheric effects. cdPM consistency is verified by examining the particle size distribution and cdPM composition. The sample is then diluted, thermally denuded and directly collected in DI water by using an impinger. The cdPM sample is size segregated by a flow field flow fractionation (FlFFF) into four size ranges (with particle diameter (nm) less than 100, 100-150, 150-200 and 200-300). The different size fractions are studied for their effect on cell viability, cellular uptake, inflammatory response, cytochrome P450 (CYP) 1 A1 mRNA induction. The biological outcomes are evaluated in A 549 human alveolar basal epithelial cells and in THP-1 cells, a pro-monocytic cell line that is differentiated to pulmonary macrophage-like cells. These results are a step towards understanding some of the interactions between the links between combustion particle physicochemical properties and health effects.

13TO.2

Identification of the Factors Responsible for the Health Effects of Atmospheric Fine Particles by Cyclone Collection Method and Exposure Experiments. TOMOAKI OKUDA, Hirohisa Takano, Akiko Honda, Shuichi Hasegawa, Takayuki Kameda, Susumu Tohno, Toshinori Onishi, Michitaka Tanaka, Masahiko Hayashi, Keiichiro Hara, Chiharu Nishita, Daiki Shishido, Yoshihiro Terui, Tsubomi Sato, Kozo Inoue, *Keio University*

Exposure to atmospheric aerosols is a serious concern for human health. Environmental quality standards have been world-widely set based on numerous epidemiological studies, and many of which have reported adverse health effects due to aerosols. However, detailed mechanisms of the cellular biochemical reactions associated with the toxicity of aerosol particles have not been elucidated well so far. Moreover, not only fine but coarse larger particles such as soil dust are considered as a potential health hazard. Generally, cell exposure studies for aerosol particles have been conducted using particulate matter collected by vibrating aerosol-loaded filters. However, the particles used for the exposure study may not be the same as those present in ambient air. Possible contamination from the filter material should also be considered. In addition, sample handling to obtain particles for exposure experiments is highly complicated and time-consuming. Besides, the amount of particles that are collected on a filter is often insufficient to perform an exposure studies. Hence, the development of techniques that allow researchers to collect a sufficient amount of aerosol particles for exposure studies without the use of filters is needed. In this study, a high-volume simultaneous sampler for fine and coarse aerosol particles was developed using the impactor and cyclone techniques. Approximately 100 mg of fine and coarse aerosol particles can be collected individually as powder form for 2-3 week sampling. The sampling device developed in this study allows researchers to collect a sufficient amount of aerosol particles for cell exposure studies without the use of filters. We collected fine and coarse aerosol particles in three cities (Yokohama, Saitama, and Fukuoka) in Japan under the CYCLEX (Cyclone collection of PM2.5 followed by Exposure Experiments) project. Chemical analysis of the collected particles has been carried out followed by cellular exposure experiment. We found particle size- and sampling location-dependent response in the results of exposure experiments.

13TO.3

Personal and Ambient Exposure of Fine Particulate Matter and Its In-Vitro Effect on Lung Cell Line: A Study for Metro City Delhi. ANANYA DAS, Nisar Ali Baig, Arun Kumar, Vivekanandan Perumal, Gazala Habib, *IIT Delhi*

The heavy metals and organic compounds adsorbed on the surface of PM may cause pro-inflammatory effects by production of reactive oxygen species (ROS) leading to respiratory, and cardiovascular illnesses. The $PM_{2.5}$ concentration in metro cities of India has crossed the alarming levels. Limited studies have reported the link of PM concentration with respiratory parameters observed with spirometer while none has reported the toxicological effect of PM on human lung cells. Therefore, this study will present the cytotoxicity, ROS and omics of PM on A549 human lung cell. The personal exposure mass was collected on five stages (PM_{10}-$PM_{2.5}$, $PM_{2.5}$-$PM_{1.0}$, $PM_{1.0}$-$PM_{0.5}$ $PM_{0.5}$-$PM_{0.25}$ and after filter) of cascade impactor (SKC, USA) at road site near main gate of Indian Institute of Technology Delhi during January to June 2017. The 6-hrs average mass concentration of PM collected on all stages was varying on monthly basis with lowest concentration was observed in March (122.2±76.5 μg/m^3) and highest (203±74.64μg/m^3) in January. $PM_{2.5}$ were also collected at urban background (15 m height) away from the roads and any other source activity. The average mass concentration of background PM was highest in January 2017 (221.9±98.6 μg/m^3) and lowest in March (84.2±17.8μg/m^3). The large variation in PM mass and its toxic components is expected to cause very different effect on lung cell viability. Therefore, this study will discuss the monthly variability in PM mass concentration and its effect on viability of human lung cell (A549). The effect of personal exposure mass of coarse (PM_{10}-$PM_{2.5}$), fine ($PM_{2.5}$-$PM_{1.0}$, $PM_{1.0}$-$PM_{0.5}$ $PM_{0.5}$-$PM_{0.25)}$ and ultrafine (After filter) particles will be presented. The lung cells exposed to 3-days composites particulate mass will be studied for cytotoxicity, ROS and omics. The concentration for both the personal and ambient were found to be more than NAAQS (National Ambient Air Quality Standards) which is set as 60 μg/m^3 for 24 hours and 40 μg/m^3 annually so this study stood essential and was performed for the first time in any metro-cities in India.

13TO.4

Seasonal Variations in Fine Particle Composition from Beijing Prompt Oxidative Stress Response In Vivo and In Vitro.

MICHAL PARDO, Fanfan Xu, Xinghua Qiu, Tong Zhu, Yinon Rudich, *Weizmann institute of science, Israel*

Exposure to air pollution can induce oxidative stress, inflammation and adverse health effects. To understand how seasonal and chemical variations drive health impacts, we investigated indications for oxidative stress and inflammation in mice and cell culture exposed to water and organic extracts from urban fine particles/PM2.5 (particles with aerodynamic diameter ≤ 2.5 µm) collected in Beijing, China. The heating season (HS, winter and part of spring) PM2.5 samples contained more pollutants than the non-heating season (NHS, summer and part of spring and autumn) PM2.5. The HS samples had high content of dissolved metals in the water extracts and polycyclic aromatic hydrocarbons (PAHs) in the organic extracts compared to the non-heating samples. An increased inflammatory response was detected in the lung and liver following exposure to the organic extracts compared to the water extracts, mostly in the HS PM2.5. While suppressed antioxidant response was observed in the lung, it was activated in the liver, again, more in the HS extracts. Nrf2 transcription factor, a master regulator of stress response that controls the basal oxidative capacity and induces the expression of antioxidant response, and its related genes were also induced. In the liver, elevated levels of lipid peroxidation adducts were measured, which correlated well with histologic analysis that revealed morphologic features of cell damage and proliferation, indicating oxidative and toxic damage. In addition, expression of genes related to detoxification of PAHs was observed. Lung alveolar cells silenced for nrf2 (siNrf2) demonstrated increased susceptibility to PM-induced cell death and a higher capacity to generate reactive oxygen species. Seahorse XFe96 Analyzer of siNrf2 cells showed involvement of the mitochondria, and a higher lipid peroxidation levels than their controls which were even more salient after exposure to PM. Altogether, the study suggests that the acute effects of PM2.5 can vary seasonally with stronger health effects in the HS than in the NHS in Beijing. These changes are attributed to the high content of PAH due to coal and biomass burning for residential heating. The signaling mechanisms of air pollution involves Nrf2 and the mitochondria.

13TO.5

Airborne Nanoparticle Release and Toxicological Risk from Metal Oxide-coated Textiles: Toward a Multi-scale Safe-by-design Approach. Paride Mantecca, Kaja Kasemets, Archana Deokar, Ilana Perelshtein, Aharon Gedanken, Yeon Kyoung Bahk, Bahareh Kianfar, JING WANG, *ETHZ/Empa*

Nano metal oxides have been proposed as alternatives to Ag nanoparticles (NPs) for antibacterial coatings. Here cotton and polyester-cotton fabrics were sonochemically coated with ZnO and CuO NPs. By varying the reaction solvent (water or ethanol), NPs with different sizes and shapes were synthesized. The cytotoxic and pro-inflammatory effects of studied NPs were investigated in vitro in human alveolar epithelial A549 and macrophage-like THP1 cells. To understand the potential respiratory impact of the NPs, the coated textiles were subjected to the abrasion tests and the released airborne particles were measured.

Very little amount of the studied metal oxides NPs were released from abrasion of the textiles coated by the ethanol-based sonochemical process. The release from the water-based coating was comparably higher. Lung and immune cells viability decreased after 24 h exposure only at the highest studied NP concentration (100 mg/mL). Differently from the ZnO NPs, both formulations of CuO NPs induced IL-8 release in the lung epithelial cells already at sub-toxic concentrations (1-10 mg/mL) but not in immune cells. Calculations revealed that the exposures of the NPs to human lung due to abrasion of the textiles were lower or comparable to the minimum doses in the toxicity tests (~0.1 µg/mL), at which acute cytotoxicity was not observed.

The results alleviate the concerns regarding the potential risk of these metal oxide NPs in their applications for the textile coating and provide insight for the safe-by-design approach.

13TO.6

Inhibition of Sub-Chronic Toxicity of Halloysite Nanotubes Aerosol by Enhancing Autophagy in Vivo and in Vitro. RUI RONG, Yongming Zhang, Qixing Zhang, *University of Science and Technology of China*

Nanoclay is the component of airborne particles that causes serious respiratory diseases. Natural halloysite nanotubes (HNTs) [1] (one dimensional aluminosilicate tubular clay) represent one of the most important nanoclays, which are available on the thousand ton scale worldwide. Among various kinds of exposure ways [2], inhalation is the actual exposure route for human to be exposed to nanoparticles in general and workplace environments. It is therefore essential to study the inhalation toxic effects of HNTs to ensure occupational and consumer safety.

In this work, we designed a nose-only inhalation device and an inhalation exposure system that could appropriately generate and characterize the exposure atmosphere. An aerodynamic particle sizer (APS) (size range: 0.5–20 µm) and fast particulate analyzer (FPA) (size range: 5–1000 nm) were utilized together in tandem to efficiently monitor the particle size and distribution. By applying this system, only the nose of the subject mice were exposed to the aerosol, which allowed for exact dosing. This newly quantitative nose-only inhalation system is of great potential for the research of airborne particle toxicity.

By using of this newly designed inhalation system we evaluated the toxicity of inhaled HNTs comprehensively for different doses (2, 15, 45 mg/m^3) and periods (1 week, 2 weeks, 4 weeks). By assessing oxidative stress, inflammatory response, and autophagy, it is found that HNTs can cause sub-chronic toxicity in mice and not recover after two weeks of post-exposure. Most importantly, we found that the toxicity of HNTs can be suppressed by enhancing autophagy. We further investigated the autophagic process on the cellular level to establish the underlying mechanism of HNTs induced autophagy. It is found that the inflammatory response were negatively regulated by autophagy in Human epithelial carcinoma (Hela) cells and alveolar macrophages (AMs) separated from bronchoalveolar lavage fluid (BALF).

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13TO.7

Development of a Computerized Nose-Only Inhalation Chamber for Nanotoxicology Study. WEI-HSUAN CHEN, Ming-Yeng Lin, Chih-Ching Chang, *National Cheng Kung University*

Considerable scientific attention has been given to the exposure of ultrafine particles (UFPs) due to its role in pathogenicity. However, the relationship between the inhalation dose and response for UFP is still not very clear, resulting in the uncertainty of the dose. One reason is that the particle generation system is not very well controlled. Here, LabVIEW was used to control the computerized nose-only inhalation chamber to a selected number concentration of the test particle. We used ultrafine carbon black (ufCB) as the model UFP. The ufCB were generated by the nebulizer and then conditioned to a temperature and relative humidity of 23.5±0.5 ˚C and 55±2 %, respectively, before entering the nose-only inhalation chamber. Preliminary studies indicate that the developed particle generation system can control the particle number concentration to within 5% of the selected number concentration (6×10^5 #/cm^3) in the inhalation chamber. The geometric mean diameter and geometric standard deviation was within 5 % of 90 nm and 1.76, respectively. We exposed the rats 6 hours a day, for a total of 5 days. There were significant increases in bronchoalveolar neutrophils, but no increase in protein leakages, and TNF-alpha and VEGF productions. Importantly, the proliferation of alveolar type II cells was significantly elevated in ufCB exposed rats, compared with those exposed to clean air. The results indicate that ufCB exposure may cause significant pulmonary epithelial cell damages, without eliciting pulmonary inflammatory response. The developed computerized nose-only inhalation chamber can benefit future toxicology and pathogenesis research.

13TO.8

Characterization of an High-Efficiency Electrostatic Precipitator Regarding Particle Size, Aerosols Flow and Particle Concentration. HARALD WIEGAND, Jörg Meyer, Gerhard Kasper, *KIT, Germany*

The air-liquid interface (ALI) provides a realistic in-vitro exposure scenario for the deposition of inhalable nanoparticles onto cell cultures for toxicological, pharmaceutical and environmental research. It is hence necessary to provide a reliable and sufficient nanoparticle dose within an acceptable time while achieving the required separation of nanoparticles from the carrier gas. For this purpose an electrostatic cross-flow ALI precipitator capable of exposing cultured human lung cells to nanoparticles is presented.

A specially developed conductivity measurement technique was used to characterize particle deposition rates as it is described in [1]. Apart from its application in toxicological research a precisely characterized ALI precipitator is capable of producing suspension of well-known particle size distribution and concentration.

Experimental
In Figure 1A a schematic of the inlet and the deposition zone is shown. Three gas flows are fed into the ALI precipitator.

The aerosol flow consists of polydisperse sodium chloride particles (20-520 nm) which is used as a surrogate aerosol for deposition rate measurements. Following the dispersion of an aqueous solution into air, the particles are charged unipolarly. The humidified flow has a relative humidity of 85 to 95 % to provide suitable conditions for cell culture experiments. In order to guarantee laminar flow conditions a sheathed flow of clean air is used. All three flows are temperature controlled. The particles are deposited in an electrostatic field (1 to 3 kV/cm) directly into the wells (Figure 1A). As the conductivity of the liquid in each well changes proportionally to the quantity of deposited salt the deposition rates can be determined [1]. For particle size dependent experiments a DMA was operated at various voltages to generate a monodisperse salt aerosol. An example of a sized aerosol is given in Figure 1B. The three main peaks at 80 nm, 120 nm and 155 nm correspond to particles in Boltzmann equilibrium carrying one, two and three elementary charges. This conditioning allows a connection between selected particle sizes and their deposition rate.

Results
First results of particle deposition characterization indicate a deposition efficiency of about 40 % of the introduced particle mass in the cell culture wells. A sufficiently narrow particle size distribution with a high concentration was generated to complete an experiments in a reasonable time. The bigger particles (>200 nm) could possibly disturb the conductivity measurements, therefore the flow velocity in the precipitation zone has to be carefully selected.

Conclusion
A deposition efficiency of about 40 % and the narrow size distribution allows particle size depended deposition rate measurements in a reasonable time. The aim is a precipitator, for which the particle deposition rate can be calculated as a function of particle size and operating conditions.

[1] Wiegand, H., Meyer, J., and G. Kasper, (2015) An electrical conductivity based method of determining the particle deposition rate in air–liquid interface devices. Toxicology in Vitro, Volume 29, Issue 5, 1100-110.

14AC.1

Characterizing Potential Aqueous Secondary Organic Aerosol Formation from Biomass Burning Emissions during 2016 FIREX Campaign. SOPHIE TOMAZ, Tianqu Cui, Yuzhi Chen, Kenneth Sexton, James Roberts, Carsten Warneke, Robert J. Yokelson, Jason Surratt, Barbara Turpin, *University of North Carolina at Chapel Hill*

Secondary organic aerosol (SOA) formation through aqueous multiphase chemistry (aqSOA) is now recognized as a significant source of SOA in the atmosphere. In-cloud aqSOA formation arises from the partitioning of water-soluble organic gases (WSOGs) into cloud water, followed by their in-cloud oxidation, subsequent formation of highly oxidized molecules, and cloud droplet evaporation leaving newly-formed low-volatility products in the particle phase.

At the global scale, biomass burning (BB) is recognized as a large source of non-methane organic compounds. Some of the compounds emitted by BB, such as glycolaldehyde, glyoxal and phenol, are known to be precursors of aqSOA. However, due to the complexity of BB emissions, most oxidized organic constituents, and particularly WSOGs, remain unidentified and may represent additional substantial sources of aqSOA.

In the present work, we collected WSOGs emitted during the combustion of several western U.S. fuels using mist chamber samplers at the Fire Science Laboratory (Missoula, Montana) as part of the 2016 Fire Influence on Regional and Global Environments Experiment (FIREX). Cloud water chemistry was mimicked through aqueous OH-initiated oxidation (H_2O_2/UV), and the composition of the samples was investigated throughout the experiment using both ion chromatography (IC) and electrospray ionization interfaced to high-resolution time-of-flight mass spectrometry (ESI-HR-TOF-MS). Aqueous OH-initiated oxidation of Ponderosa pine and Douglas fir samples revealed the formation of several highly oxidized molecules including oxalate and pyruvate, which are known aerosol components. The amount of oxalate and pyruvate reached 13-16% and 2-5% of the initial total organic carbon (TOC) content, respectively, indicating that BB emissions are a non-negligible source of in-cloud aqSOA.

During the 2016 FIREX campaign, we also investigated the chemical composition of gas-phase emissions from several fires, using a high-resolution time-of-flight chemical ionization mass spectrometer (HR-ToF-CIMS) equipped with iodide reagent ion chemistry. More than 50 oxygen (O)-containing and 15 nitrogen (N)-containing organic compounds were identified in the gas phase from BB emissions. These results were combined with the aqueous OH-initiated oxidation experimental results and data from the literature, resulting in the selection of potential precursors of in-cloud aqSOA that have not been examined in prior studies. These selected compounds were oxidized in the aqueous phase in the presence of OH radical. Aqueous OH-initiated oxidation of furan-like molecules related to BB emissions revealed the formation of small organic acids, such as oxalate, that represent up to 9 % of the TOC after 150 min oxidation. Other highly oxidized molecules were also identified by ESI-HR-TOF-MS that are likely to participate to in-cloud aqSOA formation.

14AC.2

Modeling Secondary Organic Aerosol (SOA) Formation from Biomass Burning in the Euro-Mediterranean Region during the Summer 2007. MARWA MAJDI, Karine Sartelet, Florian Couvidat, Grazia Maria Lanzafame, Mounir Chrit, Solene Turquety, Youngseob Kim, Bertrand Bessagnet, Alexandre Albinet, *CEREA, Ecole des Ponts ParisTech– EdF R&D, France*

Secondary organic aerosols (SOA) contribute significantly to the mass of organic aerosols observed in the atmosphere. SOA are formed mainly by the oxidation of volatile organic compounds (VOCs) and intermediate and semi-volatile organic compounds (I/S-VOCs). Biomass burning (including forest fire and open-field burning) releases large quantities of gases and particles into the atmosphere but SOA formation in/from fire plumes are still relatively unknown due to high uncertainties in emissions and to the complexity of the physico-chemical processes involved.

Most chemistry-transport models (CTMs) include only a limited number of VOCs which leads to a considerable underestimation of SOA concentrations. This work aims at improving the modeling of SOA formation from the main VOCs emitted by biomass burning using the CTM of the air-quality platform Polyphemus. Targeted VOCs have been selected according to their high emission factors and high SOA yields. Aromatic compounds namely benzene, phenol, cresol, catechol, furan, naphthalene, methyl naphthalene, syringol and guaiacol have been considered. Their oxidation mechanisms in gas-phase have been developed based on chamber experiment results available in the literature and implemented into the model. I/S-VOCs are usually not included in emission inventories although their contribution to SOA is probably significant. Different parameterizations have been also used to simulate the ageing of I/S-VOCs emitted by the biomass burning and implemented (single-step oxidation, multi-step oxidation and the presence of non-traditional volatile organic compounds (NTVOCs)).

The performance of the model has been finally evaluated over the European-Mediterranean region for the summer 2007 marked by severe forest fire events especially in the Balkan and Greece. Sensitivity studies on the influence of the VOCs and I/S-VOCs chemical mechanisms on SOA formation have been also performed.

14AC.3

Characterizing Chemical Composition and Evolution of Brown Carbon Organic Aerosol from Primary and Photochemically-Aged Biomass Burning Emissions during 2016 FIREX Campaign. TIANQU CUI, Sophie Tomaz, Zhexi Zeng, Yuzhi Chen, Shiva Tarun, Kenneth Sexton, Shantanu Jathar, Jason Surratt, Barbara Turpin, *University of North Carolina at Chapel Hill*

Light-absorbing carbonaceous constituents of organic aerosol (OA), referred to as brown carbon (BrC), can efficiently absorb near-UV and visible radiation, potentially altering Earth's radiative forcing and cloud formation. BrC can be emitted, formed and transformed in the atmosphere, and can contribute substantially both to OA mass and to aerosol light absorption. BrC emitted from biomass burning (BB), which is usually caused by wild and prescribed forest fires, burning of crop residues, and domestic cooking and heating, is poorly characterized. Improved molecular-level characterization of biomass burning organic aerosol (BBOA) may aid understanding of the chemical mechanisms of formation and atmospheric evolution, and help determine the impacts of BrC species on air quality and climate.

The identities, quantities, and evolution of BrC directly emitted and evolved were determined using over a hundred combustion experiments systematically performed in an exclusive indoor facility at the Fire Science Laboratory in Missoula, Montana, during the six-week Fire Influence on Regional and Global Environments Experiment (FIREX) 2016 campaign. Combusted fuels were characteristic of western North America, including Ponderosa pine, Douglas fir, Engelmann spruce, Lodgepole pine, manzanita, and chamise. Specific components of the tree/bush (e.g., canopy, litter, and duff) and mixtures of these were combusted under a variety of conditions. Two general types of combustion experiments were conducted during the campaign. For the first set, fire emissions were directly delivered through a tall exhaust stack (stack burn). In the second set, emissions were allowed to fill and mix in the large (roughly 3500 m^3) combustion room for up to several hours. In addition, primary BB emissions from certain fuel types were aged in the Colorado State University (CSU) 10-m^3 portable photochemical smog chamber to determine how photochemical reactions may alter primary BrC and/or produce secondary BrC in BBOA. Teflon filter and particle-into-liquid sampler (PILS) samples of $PM_{2.5}$ were collected from all the experiments, and then characterized at the molecular level by: (1) ultra-performance liquid chromatography (UPLC) coupled to both diode array detection (DAD) and electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (ESI-HR-QTOFMS) operated in both positive and negative ion modes, in order to chromatographically resolve BBOA constituents, with a focus on BrC components; and (2) gas chromatography interfaced with electron ionization mass spectrometry (GC/MS) with prior trimethylsilylation, for known BBOA tracers such as levoglucosan.

Several well-established BBOA tracers and BrC species from primary and aged emissions were identified, with authentic or surrogate standards that agreed with retention times and MS/MS fragments. Currently, 37 individual BrC species such as nitro-aromatics and guaiacol/styrene derivatives, were quantified from the primary emissions from six fuels. These compounds contributed up to 12% of the $PM_{2.5}$ mass. Notably, this mass fraction of BrC species varied substantially by fuel type. From the photochemical experiments, 46 BBOA species were identified that were newly formed or enhanced during photochemistry of the primary (gaseous and particle) emission mixtures initiated by hydroxyl radicals in the presence of NO_x. Most of these were BrC constituents such as nitro-aromatics. Our measurements provide insights into the role of photochemical aging on the evolution of the BBOA, including BrC, and enable us to further investigate their composition, quantities, absorption, evolution and other keys properties associated with varying fuel types and burn conditions.

14AC.4

Aromatic Volatile and Intermediate Volatility Compound Oxidation with Hydroxyl and Nitrate Radicals: Night-time SOA Formation from Residential Solid Fuel Burning Emissions. SIMONE PIEBER, Urs Baltensperger, Amelie Bertrand, Joel Corbin, Josef Dommen, Rujin Huang, Felix Klein, Nicolas Marchand, Ugo Molteni, Haiyan Ni, Jay G. Slowik, Brice Temime-Roussel, Christoph Zuth, Andre S.H. Prévôt, *Paul Scherrer Institute*

Gas-phase emissions in urban environments are often dominated by anthropogenic sources, such as combustion processes used for transport and residential heating. These emissions include monocyclic aromatics (benzene, toluene, ethylbenzene, xylenes, often collectively denoted BTEX), naphthalene and higher polycyclic aromatic hydrocarbons (PAHs), and oxygenated aromatics, such as predominantly phenolic compounds, and furans. These species are reactive towards hydroxyl radicals and have been shown to form secondary organic aerosols (SOA) induced by photochemistry. Due to their low reactivity towards ozone, oxidation of these compounds by hydroxyl radicals is both the main reactive removal and SOA formation pathway for those compounds during daytime. Their chemical processing during night-time (when hydroxyl radical concentrations are low) instead remains largely unassessed. While SOA formation from the reaction of nitrate with biogenic gases has been investigated in the past, only little information on nitrate radical initiated chemistry of anthropogenic emissions and formation of low volatility products thereof has been reported so far.

Hence, we studied the day and night-time oxidative aging of non-methane organic compounds emitted from residential solid fuel burning. We used bituminous coal to generate an emissions mix used as a model for our novel study. Emissions were diluted and injected into a Teflon smog chamber, and characterized with state-of-the-art instrumentation, including a combination of two high resolution proton transfer reaction time-of-flight mass spectrometers (PTR-ToF-MS), of which one was equipped with a fast gas-chromatography module, for the identification and quantification of the emissions. The GC module allows for the separation of isomeric compounds. In parallel we deployed a flame ionization monitor, to determine methane and the total non-methane hydrocarbons. The non-refractory particle phase was characterized with a high resolution time-of-flight aerosol mass spectrometer (HR-ToF-AMS) equipped with a PM2.5 inlet lens, as well as a thermal desorption aerosol gas chromatograph-aerosol mass spectrometer (TAG-AMS) and offline samples, analyzed with ultra-high pressure liquid chromatography electrospray ionization Orbitrap mass spectrometry (UHPLC-ESI-Orbitrap-MS). The emissions were subjected to photochemical (hydroxyl radical) and dark (nitrate radical) oxidation in the SC.

We present and compare the oxidation of those emissions and link the volatility of the precursors and their oxidation products to the observed SOA formation. Finally, we also comment on differences in the gas-phase and particle-phase products formed in the two oxidation regimes as detected by the mass spectrometric techniques.

14AC.5

Hydroxyl and Nitrate Radical Oxidation of Agricultural Reduced Sulfur Compounds in the Presence of Amines. PAUL VAN ROOY, Kathleen Purvis-Roberts, Philip Silva, David R. Cocker III, *University of California, Riverside*

Gas-phase reduced sulfur compounds, such as dimethylsulfide, dimethyldisulfide, methanethiol, and hydrogen sulfide, are known to be emitted and are present around agricultural areas. Products formed through the oxidation of reduced sulfur compounds, especially dimethylsulfide, are also thought to be important to new particle formation and particle growth over the ocean. Gas-phase amines, like trimethylamine, diethylamine, and butylamine, are also emitted around agricultural areas and are considered to be important to new particle formation. Potential sources of both these compounds in agriculture are animal waste, silage, and direct enteric emissions. While chamber studies have shown amines can oxidize to form substantial mass concentration of secondary aerosol, there have been few chamber studies focused on mass yields and aerosol properties of secondary aerosols formed through the oxidation of reduced sulfurs. Similarly, there have been no major chamber studies investigating how these two compound classes interact to form secondary aerosol. To probe the properties of secondary aerosol formed through the oxidation of reduced sulfurs in the presence of amines, a series of both single and multiple precursor experiments were conducted in a 37.5 cubic meter chamber at the University of California, Riverside. Experiments were conducted in under both dry and humid conditions utilizing either nitrate radical (300ppb) or hydroxyl radical (1ppm) as an oxidant. During single precursor experiments, 100ppb of a single amine or reduced sulfur was injected into the chamber. During multiple precursor experiments, 100ppb of a reduced sulfur as well as 100ppb of an amine was injected into the chamber. In most cases, multiple precursor experiments formed secondary aerosol mass concentrations substantially larger than either of the individual precursor experiments. For example, hydroxyl radical oxidation of methanethiol with diethylamine formed over 55 micrograms per cubic meter of aerosol while the individual precursors formed less than 15 and 10 micrograms per cubic meter, respectively. The composition of the secondary aerosol that formed during each experiment was measured using a High Resolution-Time of Flight-Aerosol Mass Spectrometer. Multiple precursor experiments tend to form more oxidized organic sulfur compounds as compared to the single precursor reduced sulfur experiments. The presence of humidity had a profound impact on the composition of the secondary aerosol formed during single precursor reduced sulfur experiments as well as multiple precursor experiments. During dry experiments organic-sulfur compounds were prone to grow in, while during humid experiments these compounds were largely absent and replaced by sulfate aerosol, likely sulfuric acid. The type of oxidant played a paramount role in the composition and mass yield of the amines. Amines oxidized by the nitrate radical often reacted quickly and formed nitrate salts; aerosol formed through hydroxyl radical oxidation of amines was more gradual and lacked nitrate salts. Surprisingly, during some multiple precursor experiments, such as trimethylamine with dimethyldisulfide, the composition of the secondary aerosol that formed was nearly identical regardless of the oxidant. This novel investigation provides insight into the important role that amines and reduced sulfurs play in the formation of secondary aerosols, especially around agricultural areas.

14AC.6

Characterization of Surface-Active Organics in Seawater and Primary Marine Aerosol Particles. AMANDA FROSSARD, Tret Burdette, Whitney Hudson, *University of Georgia*

Surface-active organics account for a minor fraction of the total organic carbon in the ocean but may have a major impact the surface tension of bursting bubbles at the sea surface that drive the production of primary marine aerosol particles (PMA). Surfactants associated with PMA may also significantly reduce the surface tension of water thereby increasing the potential for aerosol growth and cloud droplet activation. The transfer of surface-active organics from seawater and their relative enrichment in PMA remains unconstrained. In this study, PMA were produced from bursting bubbles in a high capacity marine aerosol generator. Generated PMA (gPMA) from ambient seawater and model seawater containing sea salt and surface-active organics were compared. The hygroscopic growth and number size distributions of the gPMA particles were measured using a Humidified Tandem Differential Mobility Analyzer (HTDMA). Surface-active organics were extracted from gPMA and seawater samples, and their compositions and concentrations were measured with mass spectrometry. Surface tensions and critical micelle concentrations (CMC) were quantified for the surfactant extracts, as well as the seawater. Higher surfactant concentrations were measured in gPMA from coastal and biologically productive seawater, compared to oligotrophic seawater. Surfactants extracted from coastal and biologically productive seawater directly were stronger than those from oligotrophic seawater. Photochemical reactions in the ocean mixed layer may influence surfactant properties and drive the observed variations in both seawater and gPMA surfactant concentrations over diel cycles. This work demonstrates a direct link between surfactants in seawater and those in PMA.

14AP.1

The Kinetics of Aerosol Gelation. PAI LIU, William Heinson, Rajan K. Chakrabarty, *Washington University in St. Louis*

Sol-to-gel transition is a universal phenomenon in irreversible non-coalescent aggregation systems. When the average size of aggregates reaches the length-scale of their average nearest neighbor separation, an aerosol system is said to gel–this condition is defined as the ideal gel point (IGP). Beyond IGP, the kinetics of particle growth remains elusive because of the breakdown of the governing Smoluchowski equation. In this work, we systematically study the dynamics of gelling systems in this regime using the three-dimensional off-lattice diffusion limited cluster-cluster aggregation model. Our results show that beyond IGP, the sol phase particles cease to grow without forming into gels and their corresponding normalized mass distribution remains invariant. This invariant distribution next implies that the sol-to-gel conversion of particles during a unit time is independent on particle size. Furthermore, the relationship between conversion rate and time is parameterized using a power-law, based on which analytical solutions are derived for both the decrease in the total number of sol phase particles and the increase in average mass of the gel phase particles. We conclude this work with a quantitative description on the time-evolution of the monomer fraction in gel phase.

14AP.2

Measurement of the Dynamics of Inertial, Rigid Nylon Fibers in Isotropic Air Turbulence. SOFIA KUPERMAN, Lilach Sabban, René van Hout, *Technion – Israel Institute of Technology*

Atmospheric dispersion of fibers is of importance in a variety of environmental and health related studies. For example, asbestos fibers may remain suspended in the air for a long time and when inhaled may get trapped in the lungs and cause cancer. Also, atmospheric ice crystals may resemble fibers and their orientation affects the earth's albedo.

Very few experimental data exist regarding inertial fiber dispersion in isotropic turbulent flow. Most published experimental and numerical studies investigated neutrally buoyant (inertialess) particles. These studies have found that fibres preferentially align with the stretching direction of the fluid. Lately, numerical simulations have used Jeffery's equation incorporating inertia and turbulence to study fiber dynamics. Here, rigid, inertial fibers in isotropic air turbulence were tracked using two-orthogonal digital inline holographic cinematography. The main goal of the present measurements is to gain insight into fiber length and inertial effects on their rotational and translational dynamics.

The present measurements were conducted in a turbulence chamber ($40\times40\times40$ cm^3). Isotropic turbulence was created by air jets (random frequency and phase) generated by eight woofers located at the vertices of the chamber. The isotropic turbulence was characterized by a Taylor microscale Reynolds number of $Re_\lambda = 130$, and Kolmogorov length and time scales of $\eta_k = 177$ µm and $\tau_k = 2.08$ ms, respectively. The fibers were released from the top of the chamber using a specially designed dispenser. Care was taken to ensure that the fibers were not released in clumps. A two orthogonal view, holographic cinematography system was used to track fibers in the volume of interest (VOI, $17\times17\times17$ mm^3) at the intersection of the cameras' fields of view, at the center of the chamber. The holographic cinematography system consisted of two high-speed, lensless cameras (Photron Ultima APX, 1024×1024 pixels at 2 kHz), a high-speed pulsed laser (Crystalaser, 527 nm, 10 µJ/pulse at 2 kHz), a spatial filter, collimating lens, beam splitter and mirrors. The collimated laser beams and the cameras were aligned, and to ensure time-resolved measurements, each camera acquired holograms at 2 kHz, i.e. a time separation of $0.5\text{ms} < 0.25\tau_k$. The holograms were subsequently digitally reconstructed in order to determine the time-resolved fiber tracks and their 3D orientation. Several different batches of nylon fibers with diameters and lengths ranging between $11 < D < 55$ µm and $0.5 < L < 4$ mm, respectively, were investigated. The corresponding Stokes number range, aspect ratios and length ratios were, $1.7 < St < 25$, $4.3 < L/D < 20$ and $4.3 < L/\eta_k < 23$, respectively. These measurements provide insight into the effect of inertia and aspect ratio on the mean-squared rotation rate of the fibres as well as their translational velocities, important for validating fiber dispersion models.

14AP.3

Experimental Verification of Transition Regime Aggregation Theories. Xiaoshuang Chen, Souvik Ghosh, David Buckley, R. Mohan Sankaran, CHRISTOPHER HOGAN JR., *University of Minnesota*

Aggregation in the gas phase is frequently described via either diffusion limited cluster aggregation theory (for which the diffusive Knudsen number is 0) or ballistic cluster aggregation theory(for which the diffusive Knudsen number is infinite). However, in most nanomaterial synthesis systems, the Knudsen number is not a fixed parameter; instead, is there is an evolving Knudsen number distribution function for an evolving distribution of aggregates. We have used a combination of TEM based image analysis and differential mobility analysis-aerosol particle mass analysis (with correct inversion of the two dimensional size-mass distribution function) to examine the relationship between scaling hydrodynamic radius and projected area with the number of primary particles per aggregates for aggregates synthesized via the decomposition of nickelocene in a microplasma reactor. The aggregates formed have mobility equivalent sizes in the 50-250 nm range. Scaling relationships for the hydrodynamic radius and projected area are compared to predictions based upon the result of Langevin dynamics simulations, in which the evolution of Knudsen number distribution is appropriately accounted for. Measurement inferred hydrodynamic radii and projected areas are in excellent agreement (typically within 5%) with scaling relationship predictions, suggesting these relationships can be used to infer the transport properties of aggregates in a wide range of gas phase systems. Interestingly, the scaling relationships appear to hold despite the inferred fractal dimensions of individual aggregates varying considerably (from 1.6-2.2). Furthermore, in both experiments and simulations, for aggregates of a given mass, the variations in hydrodynamic radii and projected area equivalent radii are smaller than the variation in radius of gyration. Results hence suggest caution should be exercised when employing mobility/drag based measurements to infer aggregate geometric properties (e.g. fractal dimension, radius of gyration), and that commonly inferred parameters such as the mass-mobility exponent are not strong indicators of aggregate morphology.

14AP.4

Entropy Evolution of a Coagulating Aerosol. ADAM M BOIES, Nihal El Fahim, *University of Cambridge*

Summary

The dynamics of aerosol coagulation is often dominated by the Brownian collisions motion of particles, as described by the Smoluchowski equation. During this process, the size distribution of particles changes and is well-explained by existing kinetic theory which accounts for the evolution in time of particles number density. For sufficiently long times, the kinetic theory of the coagulation process is known to reach a self-preserving size distribution. While the kinetic process is well understood, the thermodynamics associated with coagulation has received relatively little attention. Entropy, a fundamental thermodynamic property, has been employed within the informational sense to explain the evolution of particle morphology, but no study has attempted to identify the components of entropy generation with a coalescing aerosol.

Introduction

In this presentation, entropy is approached from a fundamental level using statistical mechanics and is used to analyse the thermodynamic stability of aerosol systems. First, the different forms of entropy of aerosol particles are derived and the total entropy of an aerosol system is formulated. The distribution function maximising the entropy is then derived analytically and the values of entropy for common distribution functions are calculated and compared. Finally, using different initial aerosol populations, entropy variations in time are studied using the advanced aerosol dynamics solver.

Results

We first identified the primary components of entropy generation that correspond to a loss of information relating to atomic position or momentum for each atom (or monomer) within the aerosol system. We demonstrate that entropy arises from particle parameters (kinetic movement and position) and atomic arrangement (configurational and surface) within the particle. Statistical thermodynamic expressions are derived for each component of the aerosol entropy and it is shown that the rate of entropy generation is dominated by configurational entropy.

The main findings that arise from this study are that the kinetic limited process of coagulation does not reach a maximum entropy for a given volume and number concentration, but approaches a local entropy maximum rather than a global maximum for short periods of time. The maximum entropy size distribution function for example is a combination of Dirac functions, and, for a given volume and particle number constraints, the Gumbel and Lognormal distributions exceed the self-preserving distribution in their values of entropy. This self-preserving is still observed, however, in practical cases because it is the one most compatible with the kinetics of aerosols. In a dynamic process, variations of entropy are found to be very dependent on the initial population considered. As will be shown, the entropy of a coagulating system evolves to the same final state for a given total particle volumes, but at different rates depending on the initial particle concentration and size.

Further work from the Boies group seeks to expand the analysis to include non-coalescing aerosol agglomeration, as well as aerosol processes such as charging and restructuring.

14AP.5

A Closed Form Expression for the Collision Kernel to Describe Attractive Coulombic Interactions and a Framework for Generalization to Arbitrary Attractive Potentials.

Harjindar Singh Chahl, RANGANATHAN GOPALAKRISHNAN, *The University of Memphis*

Accurate collision rate kernel models for describing collision processes in aerosol and dusty plasmas are necessary for high-fidelity engineering of synthesis reactors and for analyzing experimental data from electrical mobility analysis and Languir Probes. While the effect of strong Coulombic interactions is described accurately at conditions of infinite collisionality (continuum limit) and zero collisionality (free-molecular limit), descriptive self-consistent models in the transitiion regime and more importantly in the near-free molecular regime remain elusive. The key challenge in modeling these regimes is modeling the loss of momentum and kinetic energy of charging ions due to collisions with neutral gas molecules in their approach towards an aerosol particle or a dust grain. In the absence of viable alternatives, the free-molecular expression for the collision kernel (also known as the Orbital-Motion Limited theory) is used in instances wherein the pressure is low but not exactly zero. While the collision kernel is higher by several orders of magnitude due to increased frequency of ion-gas molecule scattering (also referred to as three body trapping or charge exchange collisions), this effect is not captured by the collision-less free-molecular expression, leading to erroneous interpretation of aerosol and dusty plasma charge distributions as well as Langmuir Probe currents. It is known that the collision kernel asymptotically approaches the free molecular limit, but an accurate expression that captures the physics is unavailable at the moment. Following prior work, we use ab initio Brownian Dynamics to infer the non-dimensional collision kernel H as a function of the electrostatic potential energy to thermal energy ratio ψE and the diffusive Knudsen number KnD. By analyzing the underlying distribution of H, we have discovered that a 3-parameter generalized extreme value distribution accurately describes the same. By analyzing the dependence of the distribution parameters on ψE and KnD, we have derived a closed form expression for the H that is valid for any ψE and KnD. This expression is tested against H calculations at values of ψE and KnD that were chosen outside the range considered here to prove its applicability at any KnD all the way up to the free molecular limit as KnD → ∞. Beyond the specific Coulombic potential considered here, a generalization to accommodate any potential is shown. This has important consequences as the abstract model of collision between two entities through a long range Coulombic interaction acting along with short range image and van der Waals, and very short range repulsion interactions (part of Lennard-Jones type potentials) model phenomena that span several fields such as aerosol science, plasma science and gas-phase physical chemistry. Lastly, a pathway to generalizing this approach to accommodate the effect of high concentration is outlined for future work in this direction to move beyond the dilute-limit approximations for systems that necessitate the same.

14AP.6

Investigation of the Contact Force Model of a Micrometer-sized Particle Impacting on a Wetted-surface. HUANG ZHANG, Qianfeng Liu, Yiyang Zhang, Shuiqing Li, Pratim Biswas, *Washington University in St Louis*

The system of a micrometer sized particle impacting on a wetted surface is usually observed in many industrial processes including additive manufacturing, 3-D printing and other technologies. Different from the millimeter grains, the particles with micrometer-sizes will experience a strong adhesion effect due to van der Waals force. Besides, the thin liquid layer on the wetted wall will supply additional cohesive and resistance influences on the falling particle. A theoretical study is carried out to depict the falling, penetrating, and bouncing process of a micrometer-sized particle. Especially, the Hamaker constant of the van der Waals force was carefully studied in considering that there is a liquid film between the particle and the surface. Various contact forces were modeled to establish a governing ordinary differential equation of the impacting particle. Besides, the evolution of the position, velocity, acceleration and restitution coefficient of the particle were determined to compare with those of millimeter sized particles. Finally, the models of the different contact forces were analyzed and compared to experimental data.

14BA.1

Capture and Inactivation of Bio-aerosols using ZnO Nanofibers. ACHARIYA SURIYAWONG, Sukanya Munthum, Varong Pavarajarn, *Faculty of Engineering, Chulalongkorn University, Thailand*

Human exposure to airborne micro-organisms has been shown to cause various health effects, including infectious diseases, acute toxic reactions and allergies. In the past decade, several outbreaks of airborne pathogens, such as Severe Acute Respiratory Syndrome (SARS) and avian flu have raised the public's concerns about the airborne micro-organisms and called for the urgent development of fast detection and effective control techniques. Filtration is one of the most widely used methods for collecting airborne particles; however, this technique alone cannot effective inactivate the collected bio-aerosols. ZnO composite has been receiving attention recently due to its properties, which are applicable in many applications, including inactivation of micro-organisms. This study synthesized ZnO/PET composite nanofiber via electrospinning technique combined with hydrothermal process and evaluated the synthesized material for their filtration efficiency and antimicrobial property. This work is divided into 2 parts: (1) investigate the influence of synthesized conditions on the physical, chemical and anti-microbial properties of ZnO/PET nanofibers and (2) evaluate the filtration and inactivation efficiencies of the synthesized materials when exposing to airborne micro-organisms. The results showed that the hydrothermal conditions play an important role on structure of the nano-fibers, average diameter of synthesized fiber and average of zinc oxide particles, chemical properties of the composites, and subsequently their anti-microbial property. The synthesized nanofibers undergone hydrothermal temperature of 200oC for 0.5hr exhibited the highest inactivation efficiency for 3 types of bio-aerosols, including B. subtilis, P. fluorescens and S. epidermidis. The fibers that exhibited the highest inactivation efficiency via AATCC standard method were evaluated for the filtration and inactivation efficiencies of airborne bio-aerosols. The results showed that the filtration and inactivation efficiencies of the nanofiber was 99.5% and 97%, respectively.

14BA.2

Technical Considerations for Device Mediated Airborne Nontuberculous Mycobacteria (NTM) Infections. SUVAJYOTI GUHA, Jon Weeks, Katharine Segars, Wolloscheck David, Ryan Fung, Delya Delavary, Kelly Bauer, Elaine Mayhall, Nicole Gillette, *U.S. Food and Drug Administration, CDRH*

Nontuberculous Mycobacteria (NTM) are waterborne opportunistic pathogens that are routinely found in water sources of hospitals and households. The prevalence of NTM associated infections is on the rise in the United States (U.S.). A review of the Medical Device Reporting (MDR) database of Center for Devices and Radiological Health within U.S. Food and Drug Administration found 253 MDRs identifying the presence of NTM in heater cooler devices (HCDs),[1] which are regularly used during certain surgeries to control the patient's temperature. Although the prevalence of NTM infections is increasing, only limited research has been conducted on device mediated airborne transmission.

Bacteria in general can aerosolize in a variety of ways – nebulization, ultrasonication and bubbling are common. Each of these modes can create different stresses on the bacterial cell walls. Specifically, for different subspecies of NTM, basic information such as size, shape, hydrophobicity, cell properties, sensitivity to relative humidity etc. is lacking. It is also not known how these factors can influence the aerosolization potential, culturability, and viability across different NTM subspecies.

This presentation will focus on two objectives: a) comparison of different modes and their influence on the aerosolization potential, and b) differences in aerosolization potential between non-biological surrogates and NTM. Our preliminary findings suggest bubbling is an effective mode of aerosolization with limited impact on NTM viability and culturability.

Reference

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14BA.3

Antibiotic Resistant Bacteria (ARB) and Antibiotic Resistance Genes (ARGs) in Air Media. JING LI, Maosheng Yao, *Peking University*

The world is facing more deaths due to increasing antibiotic-resistant bacterial infections and the shortage of new highly effective antibiotics, however the air media as its important transmission route has not been adequately studied. Based on the latest literature acquired in this work, we have discussed the state-of-the-art research progress of the concentration, distribution and spread of antibiotic resistant bacteria (ARB) and antibiotic resistance genes (ARGs) in air media, and also analyzed some future prevention and control measures. We also investigated to profile relative abundances (normalized by 16S rRNA gene) of 39 ARG subtypes resistant to 7 common classes of antibiotics including quinolones, β-lactams, macrolides, tetracyclines, sulfonamides, aminoglycosides and vancomycins in ambient particulate matter (PM) across 19 global cities. Data from the literature show that the large use of antibiotics in the medical settings and animal husbandry places has resulted in higher abundances of ARB and ARGs in the relevant and surrounding atmosphere than in urban and general indoor air environments. A number of studies have already demonstrated that ARGs can be spread by adhering to airborne particles, and researchers have also found that air media contain more abundant ARGs than other environmental media such as soil, water and sediment. It was suggested in this review that strengthening the monitoring, study on spreading factors and biological toxicity, and also research and development on pathogen accurate diagnosis and new green antibiotic are expected to help effectively monitor, prevent and control of the impacts of airborne resistant bacteria and resistance genes on both human and ecologies.

14BA.5

Aerosolization of Palytoxin in Nose-only Aerosol System. AYSEGUL NALCA, Ondraya Frick, Virginia Livingston, David Dyer, Larry Bowen, Mark Poli, *US Army Medical Research Institute of Infectious Diseases*

Palytoxins (PLTXs) are a family of extremely potent marine toxins, considered to be among the most toxic non-proteinaceous substances known. PLTXs are found in zoanthids and dinoflagellates distributed throughout tropical and sub-tropical habitats, as well as in temperate waters of the Mediterranean and Adriatic Seas. They have been isolated from seafood (fish, crabs, invertebrates) linked to human illnesses and death, and marine aerosols linked to numerous cases of flu-like symptoms, ocular irritation, and respiratory distress. Furthermore, PLTXs have been found in high concentrations in marine zoanthids (*Palythoa sp.*) commonly distributed in the home and commercial aquarium trade and they have been associated with severe respiratory reactions and corneal damage due to inadvertent contact and the presumed production of aerosols during tank maintenance and cleaning. These incidents, and many others like them, suggest that PLTXs are a family of toxins that pose a significant risk to humans through aerosol exposure. The occurrence of large annual *Ostreopsis ovata* blooms in the Mediterranean/Adriatic region, as well as the potential for toxins to be harvested in large quantities from easily obtained and cultured *Palythoa* soft corals, all argue that PLTXs represent a realistic and significant potential biotoxin threat. Therefore, we decided to characterize the aerosolized PLTX *in vitro*. PLTX congener 42-OH-PLTX (from Hawaiian *P. toxica*) and purified PLTX/42-OH PLTX from Hawaiian *P. tuberculosa* (50:50 mixture, USAMRIID) were used for sham aerosols to determine the stability of these toxins in a nose-only system. The particle size distribution (PSD) of the aerosolized test article was determined using an aerodynamic particle sizer (APS) spectrophotometer fitted with an Aerosol Diluter. The mean Mass Median Aerodynamic Diameter (MMAD) and the mean Geometric Standard Deviation (GSD) for sham exposures for purified PLTX/42-OH PLTX from Hawaiian *P. tuberculosa* (50:50 mixture, USAMRIID) and purified 42-OH PLTX from *P. toxica* were 1.66 µm, 1.73 and 1.08 µm, 2.13, respectively and these aerosolized toxin congeners had very similar spray factors.

14BA.6

Use of GREATpa System for Online Detection of Airborne Endotoxin. HAOXUAN CHEN, Maosheng Yao, *Peking University*

Endotoxins, lipopolysaccharide components (LPS) of the cell wall of gram-negative bacteria, are ubiquitous in ambient particulate matter and indoor environment. Exposure to airborne endotoxins was found to be associated with the development of asthma, bronchitis, organic dust toxic syndrome, and impaired lung function. However, current endotoxin analysis is performed mostly offline using the Limulus amebocyte lysate (LAL) assay after the air sampling process. Therefore, endotoxin dynamics in the air cannot be tracked in real-time.
Here, we developed a system (GRERATpa) that allows us to real-time monitor the airborne endotoxins. The system is composed of a high-concentrating air sampling, microfluidics, and silicon nanowire field effect transistor (SiNW FET) sensor. Before performing the experiments, the SiNW was activated and functionalized by binding anti-endotoxin antibody to the surface of nanowires via a two-step procedure. The conductance level of the SINW changes upon the binding of endotoxin to the anti-endotoxin antibody. When detecting endotoxin, the concentration level of endotoxin can be calculated using the conductance levels of the nanowire. The GREATpa system was further calibrated by using endotoxin standards and then used for the detection of endotoxin in the air in real-time. The relevant experiments are currently being conducted, but the preliminary data showed the system is working. The demonstrated technology here pioneers a new method for studying airborne endotoxins, thus providing on-line analysis of endotoxin related health risks.

Key words：Endotoxin, Online Analysis, GREATpa, Bioaerosol, Sensor

14CA.1

Optical and Thermal Measurements and Source Apportionment of TC, BC, OC, EC and CM with High Time-resolution and Comparison to Aerosol Mass Spectrometry. MARTIN RIGLER, Irena Jezek, Drinovec Luka, Janja Tursic, Kranjc Irena, Glojek Kristina, Jean-Philippe Putaud, Valerie Gros, Olivier Favez, David Green, Athanasia Vlachou, Christoph Hueglin, Yandong Tong, Giulia Stefenelli, Jay G. Slowik, Andre S.H. Prévôt, Anthony D.A Hansen, Grisa Mocnik, *Aerosol d.o.o.*

Recently developed TC-BC online method, which combines an optical method for measuring black carbon (BC) by the Aethalometer AE33, and a thermal method for total carbon (TC) determination by the Total Carbon Analyzer TCA08 was used for source apportionment of carbonaceous aerosols with high time resolution at several measuring sites around the world. TC-BC method determines organic carbon (OC) fraction of carbonaceous aerosols as OC = TC - *b*·BC, where *b*·BC is equivalent to elemental carbon (EC). The determined proportionality parameter b is region/site specific and depends to a large extent on a thermal protocol used to determine the EC fraction with the conventional OC/EC method.

TCA08 measures concentration of TC by a rapid combustion of carbonaceous matter (CM) collected on a quartz filter. Pulse of CO_2 which is created during combustion phase of the analysis is detected as a large transient increase above the CO_2 level in the ambient air used as the carrier gas. Simplicity of the analysis allow us to have high time resolution measurement and easier field deployment of the instrument as no high purity gases are needed.

TC-BC method was validated by comparing averaged high time resolved data of AE33 and TCA08 to a conventional OC/EC analysis on 24h filters using different thermal protocols (IMPROVE, NIOSH, EUSAAR2 in the following winter campaigns in Europe, Asia and N. America: Ljubljana (SI), urban background site; Loški Potok (SI), rural; Milano (IT), urban background, Paris (FR), urban background; London (UK), urban background; Zurich (CH), urban background; Magadino (CH), rural; Beijing (CN), urban; New Delhi (IN), urban; Los Angeles (CA, US), urban; Additionally, parallel measurements with aerosol mass spectrometry (AMS) allowed us to obtain hourly comparison of OM_{AMS} to $OC_{TC\text{-}BC}$.

14CA.2

Long-term High Temporal Resolution Measurements of Carbonaceous Aerosol at a Suburban Station, in Athens, Greece – Assessment of Secondary Organic Aerosol Formation. Evangelia Diapouli, Stergios Vratolis, Athina-Cerise Kalogridis, Prodromos Fetfatzis, Maria Gini, KONSTANTINOS ELEFTHERIADIS, *NCSR Demokritos, Athens, Greece*

Carbonaceous aerosol is mainly comprised of organic carbon (OC), in the form of a wide range of non-volatile and semi-volatile organic compounds, and elemental carbon (EC). These components have been found to contribute significantly to the total PM mass, at both rural and urban locations, especially in the fine particle fraction. OC may originate from a number of sources, through primary emission or secondary formation. EC is of primary origin only and is formed from the incomplete combustion of fossil fuels or biomass. Recent epidemiological studies have provided evidence that carbon-containing components may be more strongly associated with adverse health outcomes in comparison to other particulate matter (PM) components. In addition, carbonaceous aerosol has been shown to have significant impacts on the global climate change through direct and indirect radiation forcing. The present study employs high resolution data of EC/OC concentrations collected over a long-term period (5 years) in Athens (Greece), in order to provide insight into the sources and processes affecting carbonaceous aerosol in urban environments.

The measurements were conducted at the NCSR Demokritos (DEM) suburban station in Athens, Greece, during 2013-2017. Near-real time EC and OC concentrations were monitored on a 3 h basis, by thermo-optical transmittance (TOT) method, by the use of an OCEC semi-continuous field analyzer (Sunset Laboratory, Inc). The instrument was sampling at a flow rate of 8 lpm, from a $PM_{2.5}$ cut-off inlet and was equipped with an in-line parallel carbon denuder for the removal of organic gases. The EUSAAR2 protocol was applied for sample analysis. In addition, real-time data of aerosol absorption at seven wavelengths (370, 470, 520, 590, 660, 880 and 950 nm) and of equivalent black carbon (eBC) at 880 nm were derived from a 7-wavelength aethalometer (Rack Mount Aethalometer Model AE31, Magee Scientific Corp.). The aethalometer was recording every 5 min. The raw aethalometer data were corrected for the multiple scattering and shadowing effects, with the use of parallel measurements of aerosol scattering, obtained on a 1 min basis by a 3-wavelength nephelometer (Aurora 3000, Ecotech Pty Ltd). Real-time standard meteorological data were also collected. In addition, NO_x and O_3 concentration data were available from a National Monitoring Station located at around 300 m from the DEM station. Diurnal, weekly and seasonal variability of EC and OC levels, OC-EC relationships and OC/EC concentration ratios were analysed in order to assess carbonaceous aerosol levels and identify the main sources and/or atmospheric conditions responsible for the observed concentration levels. In addition, different calculation algorithms for the apportionment of OC to primary and secondary sources were evaluated. The contribution of secondary organic aerosol has been assessed and the factors governing secondary formation mechanisms have been studied. Relationships of EC-OC with other aerosol parameters (such as BC) and gaseous pollutants were studied in order to further understand the origin and characteristics of the Athens suburban carbonaceous aerosol.

Mean 24 h elemental and organic carbon concentrations over the 5-year measurement period were found equal to 0.7± 0.2 μg m^{-3} and 3.4 ± 1.5 μg m^{-3}, respectively. The corresponding OC-to-EC concentration ratios were calculated equal to 6 ± 17. High ratios during the warm period pointed towards increased photochemical secondary formation of organic carbon. The diurnal trends of OC and EC concentrations followed dissimilar patterns. EC displayed a clear morning peak (between 6 and 9 am), which may be attributed to the morning rash hours. During the cold period, both OC and EC exhibited high concentrations at night (9pm to 12 am), probably due to the shallowing of the mixing layer. Nevertheless, an enhanced increase was observed for organic carbon (as documented by the diurnal patter of the OC/EC ratio), suggesting an additional source for OC, such as condensation of semi-volatile organic compounds due to the lower night-time temperatures. The OC/EC ratio displayed also a clear day-time peak (between 12 and 15 pm) which points towards secondary aerosol formation promoted by the enhanced solar radiation. The overall results indicate low levels for the primary carbonaceous components, due to the suburban character of the site. Nevertheless, the impact by local combustion sources (traffic and domestic heating, including the use of biomass burning) is clearly shown through the seasonal, weekly and diurnal variability in the concentrations. A significant contribution from secondary organic aerosol is also documented. The results highlight the value of high temporal resolution data in the continuous efforts of the scientific community to understand the sources and processes affecting the evolution of carbonaceous aerosol components.

14CA.3

The MWAA Model as a Tool for Carbonaceous Aerosols Apportionment and as an Input for the Improvement of TOT Measurements.

DARIO MASSABÒ, Vera Bernardoni, Rosaria Erika Pileci, Silvia G. Danelli, Lorenzo Caponi, Gianluigi Valli, Roberta Vecchi, Paolo Prati, *University of Genoa and INFN Genoa, Italy*

From the local to the global scale, carbonaceous aerosols (**CA**) play a crucial role on health and climate. In urban environments CA are a major component of PM: composed of Organic Carbon (**OC**) and Elemental Carbon (**EC**), are mainly found in PM finest fractions (PM2.5 and PM1). EC can strongly absorb light, which is why, when determined using optical methods, it is called Black Carbon (BC); the OC is instead characterized by a substantial transparency in the VIS range, except for a small fraction consisting of weakly absorbing and fairly refractory organic macromolecules: the Brown Carbon (**BrC**). The BrC absorption coefficient is characterized by a greater spectral dependence ($b_{abs} \approx \lambda^{-4}$) than the BC ($b_{abs} \approx \lambda^{-1}$).

Thanks to the optical analysis of PM samples, carried out thanks to the **MWAA** [**1,2**] (*Multi-Wavelength Absorbance Analyzer* – an instrument developed at the Dept. of Physics of the University of Genoa), it is possible to derive the CA source apportionment starting from the measurement of the aerosol absorption coefficient, determined at 5-λ. Through this methodology (***MWAA model***) it is possible to quantify EC and OC coming from the combustion of fossil material (**EC_{FF}** and **OC_{FF}**) and wood (**EC_{WB}** and **OC_{WB}**) [**2**]. The *MWAA model* has recently been refined and applied to more complex situations than rural/mountain, such as PM samples collected in the very high-polluted city of Milan, Italy [**3**]. As previously demonstrated for rural sites, also in this complex situation, given by a great number of pollution sources and very stable meteorological conditions causing a huge production of secondary aerosols, **EC_{WB}** and **OC_{WB}** apportioned by the model turned out to be very correlated with **Levoglucosan**, determined in the same samples by HPLC-PAD. The optical apportionment coming from the *MWAA model* also provides a direct measurement of the Ångström absorption exponent of the BrC (αBrC), which was found to be, also in this urban environment, 3.95 ± 0.20.

The thermo-optical techniques (**TOT/TOR**) currently represent the reference method for the quantification of EC and OC. Despite their diffusion, there is still a considerable disagreement between the results obtained, since the quantification of EC and OC varies according to the thermal protocol used and by the PM composition. Furthermore, the presence in the sample of BrC can alter the "split point", as it is able to absorb the laser light (635 nm) used to monitor the transmittance during the analysis [**4, 5**]. In order to investigate how the BrC affects the EC/OC separation, and with the objective of quantifying this important fraction of the OC, a Sunset EC/OC analyzer unit has been modified in order to make possible measurements also with a 407 nm laser. At this wavelength, BrC is much more absorbent and therefore able to influence deeply EC/OC separation.

Here we present the results of the refined *MWAA model*, applied to both rural and urban PM samples, and how the results obtained through the model can be implemented in the dual-λ TOT analysis to obtain valuable information on BrC concentration.

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14CA.4

Long-Term, Continuous Aethelometer Monitoring Data Reveal Unexpected Black Carbon and Brown Carbon Sources.

K. MAX ZHANG, George Allen, Philip K. Hopke, James Schwab, Oliver Rattigan, H. Dirk Felton, *Cornell University*

Rochester, NY has one of the longest uninterrupted monitoring of light-absorbing PM in the world. A two-wavelength Aethalometer (model AE-22) has been operating continuously at an urban site since 2004. Our recent analysis of the existing data revealed some surprising findings. First, our examination of temporal patterns showed a consistent late nighttime (around 10 pm) peak of BC (880 nm) in all seasons, which was not consistent with traffic patterns in Rochester. Further analysis clearly demonstrated that the dominant wind direction for high nighttime BC almost perfectly align with a railway line near the monitoring site. It is likely that some nighttime idling and switching activities of diesel locomotives in the railway yard about 1.5 km from the monitor lead to the observed elevated BC concentrations . Second, our analysis indicated that daily mean DC (= BC(370nm)-BC(880nm)) values are statistically higher on weekend days than weekdays during summertime. Since DC has been shown a good woodsmoke (or Brown Carbon) indicator, we originally believed that the DC signals should be quite low in summertime in the absence of heating demand. Zooming into the time series of BC (880 nm) and DC reveals that spikes of synchronized PM2.5, DC and BC(880 nm) around midnight on weekend days. These results strongly suggest a non-negligible contribution of recreational wood burning to PM2.5 during summertime by source apportionment analysis. The potential sources could include camp fires, chimineas, and fire pits. Our findings support the benefits of long-term, continuous light-absorbing PM monitoring on air quality management.

14CA.5

Characteristics of Carbonaceous Aerosols at Two Major Cities Located in the Indo-Gangetic Basin. ATAR SINGH PIPAL, Ajay Taneja, Suresh Tiwari, *Dr. B. R. Aambedkar University, Agra, India*

Carbonaceous aerosol is a large fraction of atmospheric aerosols, played a crucial role in air pollution, adverse health, visibility reduction and climate effects. They constitute a significant fraction in fine particles (PM2.5), and it could be accounted for up to 40% of mass of PM2.5 in urban atmosphere. Agra, which is one of the oldest cities “World Heritage site” and Delhi, is the capital city of India; both are located in the border of Indo-Gangetic Basin (IGB) and heavily loaded with atmospheric aerosols due to tourist place, anthropogenic activities and its topography respectively. The present study was carried out at Agra as well as Delhi during winter period from Nov. 2011 to Feb. 2012 of fine particulate (PM2.5: d < 2.5 µg) and associated carbonaceous aerosols. PM2.5 was collected at both places using medium volume air sampler and analyzed for organic carbon (OC), and elemental carbon (EC). Average mass concentration of PM2.5 was 165.42±119.46 µg m-3 at Agra while at Delhi, it was ~ 27 % (211.67±41.94 µg m-3) higher as compared to Agra. Concentrations of OC and EC were 69.96±34.42 and 9.53±7.27 µg m-3 at Agra and 50.11±11.93 and 10.67±3.56 µg m-3 respectively. The OC/EC ratio was 13.75 and 5.45 at Agra and Delhi respectively. Significant correlation between PM2.5 and its carbonaceous species were observed indicating similarity in sources at both sites. In the case of POC, similar concentrations were observed at both places but in the case of SOC higher over Agra by 24 in comparison to Delhi, it is due to the high concentration of OC over Agra. Secondary organic aerosol (SOA) was 42% higher at Agra than Delhi which confirms the formation of secondary aerosol The SOA contribution in PM2.5 was also estimated and was ~32% and 12% at Agra and Delhi respectively. Being high loading of fine particles along with carbonaceous aerosol, it is suggested to take necessary and immediate action in mitigation of the emission of carbonaceous aerosol in the northern part of India.

14CA.6

Characteristics and Origins of Carbonaceous Aerosols at an Urban Site of Qatar Peninsula. WASIM JAVED, Bing Guo, Minas Iakovides, Qi Ying, Euripides G. Stephanou, *Texas A&M University at Qatar*

Doha, the capital of Qatar, has the world's twelfth highest levels of atmospheric particulate matter (PM). However, research has been scarce on the level, composition and sources of aerosol pollution in the city. In this study, mass concentrations of PM, elemental carbon (EC) and organic carbon (OC) fractions as well as ninety individual organic compounds, grouped into PAHs, n-alkanes, hopanes and steranes, were measured in $PM_{2.5}$ and PM_{10} filter samples at an urban site in Doha, aiming to establish concentration profiles and quantify the contributions of major sources in the area. Three sets of 24-hr filter samples were collected for each $PM_{2.5}$ and PM_{10} mass determination, EC/OC analysis and organics speciation from May to December 2015. The real-time mass concentration of PM and black carbon (BC) were also measured by using a DustTrak aerosol monitor and a 7-channel Aethalometer, respectively.

The 24-hr average PM_{10} and $PM_{2.5}$ concentrations (±SD) were 145±70 and 40±15 $\mu g\ m^{-3}$ respectively, about 2-3 times higher than the WHO standards. The average EC in $PM_{2.5}$ and PM_{10} were 2.61±1.1 and 3.0±1.3 $\mu g\ m^{-3}$ and that of OC were 1.78 ±1.14 and 6.97 ±4.2 $\mu g\ m^{-3}$, respectively. Temporally, PM and BC mass concentrations exhibited well-defined diurnal variations, comprising of a single prominent peak occurring in the morning (6-7am), and were always higher by a factor of about 1.5 during nighttime than the concentrations during daytime. The average $PM_{2.5}/PM_{10}$ ratio was 0.30, a value that is typical of urban sites affected by the desert environment, suggesting the dominance of coarser particles.

It was found that total carbonaceous contents accounted for 10 to 18% of the PM mass. A dominant fraction (90%) of EC was associated with $PM_{2.5}$ particles, while about 71% of OC was present in coarser fraction ($PM_{2.5\text{-}10}$), out of which around 68% is in the form of secondary OC. The n-alkanes were the most abundant group followed by PAHs and hopanes, while steranes concentration was the lowest. Long-chain n-alkanes (C25 to C35) accounted for about 90% of the total analyzed n-alkanes with a predominance of odd carbon numbered congeners (C27-C31). High molecular weight PAHs (5-6 rings) accounted for 63% of the total measured PAHs, while Benzo[b+j] fluoranthene (Bb+jF) was the most dominant species. PAHs were mainly (80%) associated with $PM_{2.5}$ size fraction. The hopane and sterane tracers also confirmed the contribution from petroleum sources (vehicles and refineries).

Remote sources and local sources both contributed to the carbonaceous aerosols observed at the site, depending on the wind speed and direction. Two pollution episodes were observed during the sampling period that provided additional insight into the transport mechanisms and potential sources of these organic pollutants. The PMF model and diagnostic ratios/indices all suggested that vehicular emissions were the primary pollution sources. In descending order of importance, PMF-derived organic sources were fugitive dust and gas-phase fugitive emissions (32.9%), gasoline engine emissions (26.7%), diesel engine emissions (20.1%), petrogenic/biogenic emissions (12.9%) and waste burning (7.4%). Because of site's location relative to the city, local vehicular and fugitive emissions were predominant during south-easterly winds from urban areas, while long-distance petrogenic/biogenic emissions were particularly significant under prevailing north-westerly strong-wind conditions.

This first report regarding the compositional profile of carbonaceous aerosols and their sources in Doha provides information that can be used to monitor trends over time, identify primary sources of pollutants, evaluate health and environmental consequences and finally initiate pollution mitigation strategies.

14DU.1

Understanding Early Stage Processes during Pulverized Coal Combustion in a Two-stage Flat Flame Burner. DISHANT KHATRI, Adewale Adeosun, Akshay Gopan, Zhiwei Wang, Richard Axelbaum, *Washington University in St. Louis*

In pulverized coal burners, coal particles transition from a short period of locally reducing environment, caused due to the fast release of volatiles from a dense region of coal particles, to an oxidizing environment. This “reducing-to-oxidizing” transition can influence combustion processes such as ignition, particulate formation, and char burnout. Traditionally, fundamental studies on coal combustion have been conducted in systems which neither capture the “reducing-to-oxidizing” transition nor the high a heating rate of practical combustors. In this work, the formation and evolution of sub-micron particles are investigated in a novel two-stage flat flame burner that simulates the “reducing-to-oxidizing” transition and with heating rates on the order of 105 K/s. The particle size distribution (PSD) of the sub-micron particles, and their composition are measured using SMPS and SEM-EDX, respectively. Measurements are carried out under both an oxidizing environment (20% oxygen) and a “reducing-to-oxidizing” environment at two different nominal gas temperatures (1300 K and 1800 K), and three residence times (15, 30 and 60 ms). To differentiate between soot and mineral matter, the SMPS is operated in a tandem fashion, with a high-temperature furnace between the two SMPS measurement locations. The furnace is supplied with a sufficient amount of oxygen to burn off soot in the sampled aerosol stream. The results, including the difference between the oxidizing and reducing-to-oxidizing environments, will be discussed.

14DU.2

Excessive Air Pollution from Carbon-Neutral Fuels. Chunshui Lin, Colin O'Dowd, Darius Ceburnis, JURGITA OVADNEVAITE, *National University of Ireland Galway, Ireland*

Emissions of ambient particulate matter (PM) from the power-generation, transport, and industry sectors have been the main target of most mitigation policies, leading to substantial technological improvements along with pollutant emission reductions. However, residential PM emissions are subject to little control, even in developed countries, and represent a potentially-significant source of PM which should be taken into account in policy making. In this study, we explored PM levels during wintertime in Dublin, Ireland, in the context of peak PM concentrations encountered, frequency of exceedance of the WHO $PM_{2.5}$ daily limit (25 $\mu g/m^3$), and the main sources of PM during these exceedance periods. Positive matrix factorization (PMF) with the multi-linear engine (ME-2) has been applied to the organic matrix to quantify the contribution from different sources. We show that under polluted conditions, carbonaceous (organic matter and black carbon) aerosol prevails over historic inorganic species like sulphate and nitrate, contributing from 60% to 90% to the PM1 mass, and, in spite of common believes and expectations, the source apportionment exposed that a staggering 70% of the particulate pollution can arise from <4% consumption of solid fuels (peat and wood), often promoted as 'slow renewable', 'low-carbon' or 'carbon-neutral' biomass. Furthermore, our results suggest that even modest increases in consumption of current 'green' marketed fuels will have a disproportionate impact on the frequency of extreme pollution events and our endeavours towards cleaner air with the most extreme consequences on developing economies, such as India's or China's, due to already existing dependency on biomass as an important energy source.

14DU.3

Emission Behaviors of PM10 during Combustion of Pre-Treated Straw and Co-Combustion with Pulverized Coal.

WENYU WANG, Chang Wen, Ying Zhou, Changkang Li, Minghou Xu, *Huazhong University of Science and Technology, China*

At present no study was made to compare the effect of various thermal pretreatment methods of biomass on the emission behaviors of PM_{10} from biochar combustion, let alone the co-combustion of biochar with coal. The highlight of this article is the effect of thermal pretreatment, i.e., torrefaction (300°C), slow pyrolysis (500°C) and hydrothermal carbonation (240°C), on the emission reduction of PM_{10} generated from the combustion of biochar and its co-combustion with steam coal. Straw, as a typical and widespread agricultural biomass in China, was collected as raw materials.

The emission reduction of PM_{10} is explored via the combustion of starw and its biochars and their co-combustion with coal in a drop tube funace (DTF) at 1400°C. Compared with straw, the fuel properties of biochars are enhanced to some extent, varying from different pretreatments. During pretreatments, almost all alkali and alkaline earth metallic (AAEM) remains in T-300 or S-500 while about 10%~65% AAEM (espiclliay for K, only 10%) stay in H-240. Also, the retention of Cl is ~68%, ~58%, ~16% respectively for T-300, S-500 and H-240.

The above difference among three pretreatments may cause large discrepancy on the content of vaporized species and the generation of PM_{10}. Compared with raw straw, the emission reduction at each size range ($PM_{0.3}$, $PM_{0.3\text{-}1}$, $PM_{1\text{-}10}$) during single combustion (ash-based) are ~55%, ~55%, ~16% respectively under torrefaction, ~67%, ~56%, ~40% respectively under slow pyrolysis, and up to ~94%, ~90%, 70% respectively under hydrothermal carbonization, hydrothermal carbonization exerts the largest reduction on PM_{10} emission. Furthermore, based on equal energy input, compared with straw (single combustion), torrefaction still shows 12% of emission reduction at $PM_{0.3}$, and the advantage of H-240 on the emission reduction of PM_{10} is still encouraging, even up to 92% at $PM_{0.3}$, while S-500 already exhibits negative effect. As for blended combustion (ash-based), only hydrothermal carbonization still exhibits great advantage on the emission amount of PM_{10}, and the excellence of it gradually decreases as the increase of coal in the blend proportion. But compared with theoretical value calculated from the addition of single combustion of biomass and coal, experimental value from co-combustion exhibits great advantage on the emission reduction at PM_1, due to the capture of AAEM by kaolin in coal. However, advantages gradually disappear in the order of straw > T-300 > S-500 > H-240 for each blend ratio. The emission reduction on $PM_{0.3}$ whether for single combustion or co-combustion for straw and kinds of biochars is linearly related to the Cl content in materials. Generally, it appears that the more AAEM and Cl is released during thermal pretreatment, the less the PM_1 is generated during single combustion of biochars, and meanwhile, the less the emission reduction ratio via co-combustion is.

14DU.4

Comparison of Charge Fraction and Electrostatic Precipitation of Fly Ash from Combustion of India, US and China Coal Seams. ZHICHAO LI, Pratim Biswas, *Washington University in St Louis*

Fly ash in coal combustion exhaust gas is a major source of fine particulate matter in atmosphere in India, US and China, whose coal consumption accounts for more than 70% of world coal use (EIA 2016). In addition, fine particles have much higher tendency to escape common particle control equipment and discharge into the atmosphere. To better understand fine particle formation in coal combustion and more effectively control particle emission, it is imperative to explore the characteristics of fly ash from the combustion of coal seams widely used in different countries and their impacts on particle removal.

Electrostatic precipitator (ESP) is regarded as one of the most popular industrial particle emission control technology due to its high mass collection efficiency, capability to collect particles with diverse composition and long-term reliability. It needs to be noted that fly ash particles in combustion exhaust gas have been reported catching significant amount charges (Maricq 2004; Suriyawong et al. 2008), which might influence the particle charging process in the ESP and its capture performance (Li et al. 2016). These findings indicate that knowing charging status of fly ash is informative for better design and control of ESPs.

This study experimentally examined the size distribution, charged fraction and resistivity of fly ash from the combustion of coal from India, US, and China. The penetration of particles in a lab scale cylindrical ESP as a function of size was also measured. Because the capture efficiency is governed by complex non-linear relations, a machine learning regression method was employed to predict the capture efficiency of ESP with particle size, number concentration, applied voltage, ash resistivity, charged fraction as input variables. This work will provide novel insights for ESP modeling, design and operation.

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14DU.5

The Effects of Pressure on Alkali and Alkali Earth Metals in Particle Matter Generated from a Lab-Scale POFBC. JIA WANG, Lunbo Duan, Yuanqiang Duan, Xuebin Wang, Yong Yan, *Southeast University, China*

As a promised CO2 capture technology, pressurized oxy-fuel combustion has unrevealed characteristics on particle matter emission. Hence, a 10kWth lab-scale pressurized oxy-fuel fluidized bed combustor (POFBC) with continuous fuel feeding system and electrical low pressure impactor (ELPI) has been established and operated at 0.3 and 0.5MPa. This work focus on the alkali and alkali earth metals (AAEM) in particle matter formed under air and O2/CO2 atmosphere at elevated pressures. It is found that Na shows obvious gasification in all experimental conditions while K shows an identifiable enrichment in submicron particles only when the temperature and pressure reach the threshold. As a result, the climax of particle concentration of Na is located near 0.1µm compared with K whose climax is located near 1µm. The increasing pressure promotes the release of both Na and K from the coal by enhancing the char temperature. Mg and Na seem to share a consistent trend at high pressure, indicating Mg is released to the gas phase in pressured combustion. The content of Ca increases gradually with the increased particle diameter due to the fragment of ash during the combustion process to some extent.

14DU.6

Numerical Study on Evaporation of Inherent Minerals during Combustion of a Char Particle. SIBO QU, Haiming Wang, Changfu You, *Tsinghua University, China*

A large number of experimental studies were performed to investigate the formation of ultrafine particles during combustion of pulverized coal. An evaporation-nucleation-coagulation mechanism has been established to describe this process.

A theoretical model, considering heat and mass transfer between the particle and the surrounding gas, has been developed in transient conditions to study the kinetics of evaporation of inherent minerals, the trend of particle size and ash content evolution, with allowance for the temperature distribution in particle. A comprehensive model for the prediction of the combustion of a char particle includes combustion model and inherent minerals release model in turn. Combustion model is composed of ash sub-model, intrinsic kinetics sub-model, diffusion sub-model and heat balance sub-model. Ash sub-model is mainly used to calculate the evolution of ash film thickness, and the ash content, based on the law of conservation of mass. Intrinsic kinetics sub-model and diffusion sub-model is mainly used to calculate the evolution of coal core size, considering the effect of ash and porosity in the char particle, the overall burning rate, consisting of the combination of the internal and external burning rates of the char.The heat released through char oxidation in the char core is transferred to the ash film through conduction, and then is transferred to the surroundings through convection and radiation. Considering the radiation heat transfer, convection heat transfer, and conductive heat transfer, the particle temperature are computed in heat balance sub-model. Iron and alkali metals is distributed on the surface of particle with coal ash separate out during combustion, and then into the surrounding gas. Based on the law of conservation of mass and energy between solid and gas, and the surface ionization controlled by iron and alkali metals content in coal ash, inherent minerals release model is set up.

The experimental data of iron and alkali metals release in coal ash are compared with theoretical results. Results indicate that this approach permits to predict the extent of evaporation of inherent minerals from a mineral porous matrix.

14HA.1

Diesel Engine Exhaust Particles: Science, Regulations and Technological Developments Leading to Cleaner Emissions.

ROGER MCCLELLAN, *Private Consultant*

This presentation will review health issues associated with diesel exhaust emissions over the past century. Emphasis is given to research by the author and colleagues over the past four decades that have influenced regulations and technological developments leading to contemporary diesel engines with exhaust emissions with minimal health impact. The compression-ignition, internal combustion engine, known as the Diesel engine for its inventor, Rudolph Diesel, is a key contributor to modern industrial society. Concern developed post-WWII for exhaust impairing visibility and causing respiratory tract and eye irritation. In the 1970s, concern increased over the potential for diesel exhaust particle exposures to cause lung cancer with the finding that extracts of respirable diesel exhaust particles contained polycyclic hydrocarbons and were highly mutagenic in microbial assays. The Lovelace Inhalation Toxicology Research Institute (ITRI) took a lead role in conducting lifespan studies with rats exposed to exhaust from circa 1980 diesel engines. They found that chronic exposure to 3500 or 7000 µg/m3 of diesel exhaust particles caused lung cancer, findings soon confirmed by investigators in Germany, Switzerland and Japan. Later, studies showed exposure to carbon black particles, with no absorbed hydrocarbons, produced a similar increase in lung cancer raising questions as to the relevance of the rat findings for assessing human hazards. These findings were key to the International Agency for Research on Cancer (IARC) (1987) classifying diesel exhaust as a “probable human carcinogen.” Heightened concern for exhaust exposure causing adverse health effects led to issuance of stringent emission standards. The IARC finding also stimulated new epidemiological studies. The Diesel Exhaust in Miners Study (DEMS) conducted by scientists at the US National Institute of Occupational Safety and Health and National Cancer Institute studying 12,000 workers in non-metal mining operations through 1997 found an increased lung cancer hazard in workers exposed to diesel exhaust pre-1982. DEMS investigators used estimates of Respirable Elemental Carbon (REC) extrapolated from CO measurements as markers of exposure. DEMS findings were key to IARC (2012) classifying diesel exhaust as a “human carcinogen.” The author and colleagues replicated the original DEMS analyses and, then, extended the original analyses. The extended analyses used alternative REC exposure estimates developed based on Horse Power (HP) of diesel equipment used, REC emissions per HP and mine ventilation. Use of these exposure metrics and control for radon exposure resulted in diminished estimates of the association between diesel exhaust exposure and lung cancer. Moreover, the effect was only significant in a mine with limited ventilation and use of large diesel-powered haul units. To meet the stringent emission standards introduced post-2000, major advances were made in diesel engine technology and fuels. These advances resulted first, in reduced particulate emissions and, later, reduced emissions of nitrogen oxides. ITRI (2015) conducted lifespan studies with rats exposed to diesel exhaust from new-technology heavy duty engines equipped with an exhaust after-treatment system that reduced particulate emissions to near zero meeting EPA 2007/2010 standards. No excess lung cancer was observed. Modest respiratory tract lesions associated with NO2 exposure were observed, as expected, since the engines used were not equipped with NO2 reduction systems. These results illustrate the positive impact of improved engine design, ultra-low diesel fuel, exhaust after-treatment systems and electronic controls to eliminate the lung cancer hazard that may have existed for old technology diesel engines. In conducting risk assessments for diesel exhaust exposure, it is important to recognize the recent substantial changes in particulate exhaust emissions associated with improved technology. This is an example of the role of aerosol science as an important enabling science in developing diesel technology with reduced potential for health impacts.

14HA.2

Cyclic Siloxane Oxidation over North America: Quantifying the Strength, Properties, and Lung Cytotoxicity of Widespread Silicon from Personal Care Products. Nathan Janechek, Benjamin King, Rachel Marek, Andrea Adamcakova-Dodd, Traci Lersch, Kristin Bunker, Gary Casuccio, Kaj Hansen, William Brune, Peter Thorne, Keri Hornbuckle, Jennifer Fiegel, CHARLES STANIER, *University of Iowa*

Cyclic volatile methyl siloxanes (cVMS) are anthropogenic chemicals present in a range of consumer personal care products such as antiperspirants and lotions. They are highly volatile, but rather non-reactive – and thus found in high concentrations in indoor environments, and then are transported long distances through the atmosphere. A major removal pathway for these silicon-containing gases is reaction with the OH radical, which has been recently shown to yield secondary Si-containing aerosol compounds in addition to the established gas phase products. To investigate this further, we integrate research on the source, environmental loading, transport, and potential health impacts of this compound class. Specifically, a series of related laboratory and modeling investigations were performed. These include laboratory aerosol generation in an Oxidation Flow Reactor (OFR), physical and chemical particle characterization, *in vitro* lung cytotoxicity studies, and modeling using the Community Multiscale Air Quality (CMAQ) atmospheric transport/chemistry model.

While the parent compounds such as decamethylcyclopentasiloxane (D5) have been well-studied for potential health and ecological impacts, the oxidation products and potential aerosol species have received much less attention, with almost no ambient measurements or experimental physical property data. We generated Si-C-O aerosols by supplying D5 to an OFR. The particles were characterized for concentration, aerosol yield, size, morphology, volatility, individual particle chemical composition, and CCN formation potential (using a DMT-CCN or Droplet Measurement Technologies Cloud Condensation Nuclei Counter).

Aerosol yield sensitivity to D5 and OH concentrations, residence time, and seed aerosols were analyzed. TEM-EDS and STEM-EDS analysis show spherical particle morphology for primary particles, elemental composition consistent with aerosols derived from cyclic siloxane sources, and aggregate formation. Measured aerosol yields were 20-50% with typical aerosol concentrations 300,000 particles cm^{-3}, up to 200 µg m^{-3}, and diameters of 30-90 nm. Particles sized 10-110 nm did not experience any significant reduction in diameter after being heated up to 200°C suggesting low volatility. Particles exhibited slight hygroscopic behavior with calculated effective kappa parameters ranging between 0.006-0.02 which is comparable to the lower range of previously reported secondary organic aerosols. Smaller particles were found to have increased CCN potential, suggesting the aerosols are non-homogenous with smaller particles likely more oxidized. Acute exposure cellular toxicity was tested by exposing A549 lung epithelial cells to the generated aerosols using an *in vitro* air-liquid interface exposure system. No significant difference in cell viability could be attributed exclusively to the aerosol species and no increase was observed in biomarkers of inflammation and oxidative stress.

Three cVMS compounds and their oxidation reactions were added to the CMAQ model. Typical concentrations, seasonal variability, spatial patterns, and vertical profiles were quantified at 36 km spatial resolution over North America during four separate seasons. Typical model concentrations showed parent compounds were highly dependent on population density as cities had monthly averaged peak D5 concentrations up to 432 ng m^{-3}. Peak oxidized D5 concentrations were significantly less, up to 9 ng m^{-3}, and were located downwind of major urban areas. Model results were compared to available measurements and previous simulation results. Parent compound concentrations in urban and peri-urban locations were sensitive to transport factors, while parent compounds in rural areas and oxidized product concentrations were influenced by large-scale seasonal variability in OH.

Key uncertainties with cVMS aerosol production is the yield of aerosol and semivolatile compounds at ambient OH concentrations, and the chronic health effects of the particles. This work only addressed yield at elevated reactant concentrations, and acute *in vitro* health effects.

14HA.3

Daytime and Nighttime Particulate Matter Toxicity in an Urban City. TING ZHANG, Maosheng Yao, *Peking University*

Human exposure to particulate matters, especially ultrafine particles, can cause a wide range of diseases. However, toxicity of particles during the day and night can be quite distinct from each other since there might be some very different chemical reactions occurring. Size-fractionated (from 0.01µm to 18µm, in 13 size ranges) particulate matter samples were collected using NanoMoudi in daytime and nighttime in Beijing from September 11th to 14th, 2017. Dithiothreitol (DTT) assay was used to evaluate the oxidative potential of ambient particles. The result showed that the PM toxicity in nighttime particles was significantly higher than that in daytime for certain size ranges. Basically, both for the daytime and nighttime, oxidative potential was found to have increased with decreasing size. These results indicated that PM related health effects could be different between daytime and nighttime, and suggest a need to especially protect people from PM exposure during the night.

14HA.4

Spatial and Temporal Variability in Chemical Composition of Fine Particulate Matter and Human Health Impact Assessment for the Megacity of Karachi, Pakistan. Lurie Kelly, HAIDER KHWAJA, Shedrack Nayebare, Zafar Fatmi, David Carpenter, Daniel Malashock, Azhar Siddique, Kamran Khan, Mirza M. Hussain, Fida Khatib, *Wadsworth center, University at Albany*

Karachi, Pakistan is one of the largest and most polluted metropolitan city in southeast Asia. Air quality was assessed 24-hour fine-particulate matter ($PM_{2.5}$) samples collected from two sites, Korangi (industrial/residential) and Tibet Center (commercial/residential). Spatial and temporal characteristics and sources of pollution were evaluated from August 2008 through August 2009 using samples analyzed for $PM_{2.5}$, black carbon (BC), trace metals, and water-soluble ions. Enrichment factors were calculated, and a receptor model was used to identify anthropogenic and natural source contributions. $PM_{2.5}$ concentrations exceeded the WHO Guideline of 20 $\mu g/m^3$, ranging from 30 to 279 $\mu g/m^3$. The average for Korangi (102 $\mu g/m^3$) was greater than that for Tibet Center (77 $\mu g/m^3$). Average $PM_{2.5}$ concentrations were higher in the winter, suggesting increased burning and decreased air dispersion. Enrichment factors suggest abundant seasonal contributions of trace metals from anthropogenic activities. Concentrations of pollutants were higher at the Korangi site as compared to the Tibet Center, indicative of emissions from industrial activities near the site. Positive Matrix Factorization (PMF) was utilized to quantify sources of ambient $PM_{2.5}$. The identified sources and their percent contributions for Korangi and Tibet Center sites, respectively, are oil combustion (25% and 21%), soil and urban dust resuspension (28% and 25%), vehicular emissions (23% and 5%), sea spray (13% and 26%), and industrial emissions (11% and 23%). Human health risk assessments and impacts were evaluated and identified major air pollution concerns for Karachi, Pakistan, highlighting the need for stringent laws on $PM_{2.5}$ emission control to protect human health and the environment.

14HA.5

Relationship between Aerosol Composition and Sources and Their Oxidative Potential in Central Europe. KASPAR RUDOLF DÄLLENBACH, Gaëlle Uzu, Ivan Kourtchev, Laure-Estelle Cassagnes, Alexander Lucas Vogel, Giulia Stefenelli, Athanasia Vlachou, Jay G. Slowik, Jean-Luc Jaffrezo, Markus Kalberer, Josef Dommen, Urs Baltensperger, Imad El Haddad, Andre S.H. Prévôt, *Paul Scherrer Institute / University of Helsinki*

Epidemiological studies identified increasing particulate matter (PM) concentrations as a reason for elevated mortality even at concentrations below regulatory thresholds. For 2017, exposure to ambient PM was among the 5 leading mortality risk factors causing up to 4.33 million deaths worldwide (Lelieveld et al., 2017; Cohen et al., 2017). Compounds present in PM such as trace metals and organic compounds can carry/produce reactive oxygen species (ROS) upon inhalation of PM and further oxidize target molecules in the body leading to oxidative stress. It is hypothesized that such oxidative stress is a key variable in explaining the observed adverse health effects. The ability of PM to induce such oxidative activity, termed oxidative potential (OP), has been put forward as a measure closely related to biological responses. It is expected that PM's chemical composition is relevant in predicting its impact on human health.

In this study, we assess the spatial and temporal variability in the chemical composition of particulate matter < 10 µm (PM10) and study the association between OP and the different PM10 sources. We quantified the organic (OA) and inorganic (EC, NH_4^+, NO_3^-, SO_4^{2-}, trace metals) constituents of PM10 as well as the OP (three complementary acellular assays: dithiothreitol (DTT), ascorbic acid (AA) and dichlorofluorescein (DCFH)) at various sites in central Europe (rural background, wood burning influenced, traffic influenced). We use an aerosol mass spectrometer in combination with positive matrix factorization to quantify the sources of organic aerosols collected on offline filter samples and analysed them at a molecular level with ultra-high resolution mass spectrometry (Orbitrap-MS). We demonstrate that the factors governing air quality are region-specific. Coarse vehicular wear, the dominant source of trace metals, is strongly enhanced in urban areas. The winter-time OA pollution in alpine valleys is driven by primary organic aerosol from wood burning emissions (BBOA) and at the other sites a largely non-fossil SOA factor correlating with anthropogenic secondary inorganic species is dominant. We observe the production of mainly non-fossil SOA in summer, following the increase in biogenic emissions with temperature. The predominance of highly oxygenated compounds with monoterpene related carbon backbone (carbon number 8-10, H:C ratio ~1.5) observed with Orbitrap-MS for summer samples suggest that OA during this period is dominated by biogenic SOA. We determined the contribution of the aerosol sources/components to the OP. Aerosol's OP activity per mass quantified in this study provides reliable information for predicting ROS exposure levels for populations. We will present this thorough assessment of local and regional sources affecting air quality and human health.

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14HA.6

In Vitro Toxicity of PM Collected at Different Sites in Switzerland: Correlation between Chemical Composition and Toxicity. LAURE-ESTELLE CASSAGNES, Zaira Leni, Kaspar Rudolf Dällenbach, Gaëlle Uzu, Andre S.H. Prévôt, Urs Baltensperger, Jean-Luc Jaffrezo, Imad El Haddad, Marianne Geiser, Josef Dommen, *Paul Scherrer Institute*

Outdoor pollution is estimated to be responsible for more than 4.3 million premature deaths per year worldwide [1]. However, the link between particle properties and different adverse effects is not yet resolved. There is an urgent need to support epidemiological evidence by experiments aimed at determining which particle properties and which biological responses are the most crucial for disease development and susceptibility to air pollution. It has been shown that in the presence of antioxidants, trace metals and organic compounds, like quinones, may induce redox cycling in pulmonary cells and thereby increase reactive oxygen species (ROS) production [2]. We explored the relationship between particulate matter (PM) chemical composition and adverse effects on normal and diseased human airway epithelia at the molecular level with a focus on the interactions of particles with the inner surface of the lungs and the impact of ROS thereon.

Two model compounds were tested: a) copper (CuII) - originating from non-combustion traffic sources - and b) 1,4-naphthoquinone (1,4-NQ) – a surrogate representing redox active organic molecules emitted during combustion or produced by photochemical reactions of polycyclic aromatic hydrocarbons. These were applied to the air liquid interface (ALI) of normal and diseased differentiated human bronchial epithelia (HBE). Then, PM_{10} and $PM_{2.5}$ winter and summer filter extracts from urban and rural sites in Switzerland were deposited onto the ALI of HBE cell cultures. For exposure experiments, different biological endpoints including: cytotoxicity, release of (pro) inflammatory mediators (IL6 and IL8) as well as gene expression of selected pathways leading to inflammation, DNA damage, response to oxidative stress, apoptosis and senescence response, were assessed.

In parallel, the oxidative potential (OP) of the filter extracts was estimated by 3 assays: dithiothreitol, DTT; dichlorofluorescein, DCFH ; and ascorbic acid, AA.

1,4-NQ induced a high cytotoxicity, especially in diseased epithelia, while CuII showed less toxicity. The combination of 1,4-NQ and CuII revealed a synergistic effect regarding cytotoxicity and IL8 release. Exposure of filter extracts showed a very high sensitivity of cystic fibrosis epithelia with up to 60% cytotoxicity. The cytotoxicity variability within our dataset will be compared to source apportionment results for the organic aerosols (OA, AMS), to the OP data and to trace metals content (ICP-MS). We will discuss the role played by the PM compounds in the redox cycling at the surface of the lungs as well as the sources responsible for the adverse effects to the bronchial epithelia.

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14LC.1

Extracting Air Quality from Photographs. Batsal Pudasaini, Joseph Skufca, Sumona Mondal, Natasha Banerjee, Jan Scrimgeour, Mark Kanaparthi, SURESH DHANIYALA, *Clarkson University*

Understanding the effects of aerosol particles on human health is made challenging by the lack of high-resolution air quality data. Globally, $PM_{2.5}$ monitoring sites are limited in number, as they require extensive manpower and equipment to operate. This research takes a physics-based approach in estimating $PM_{2.5}$ by analyzing photographs from different locations. A background image is impacted by the presence of aerosol, because of a combination of particle scattering and extinction of light. We develop a governing equation that relates camera signal to the properties of aerosol, the incident light, and the image being captured. From inversion of this integral equation, we establish an expression for turbidity and estimate $PM_{2.5}$ from these measurements. Using 3-years' worth of images captured from a camera at a fixed location (downtown Chicago), the calculated turbidity is compared against actual $PM_{2.5}$ data from nearby EPA monitoring sites. It is observed that on average, turbidity and $PM_{2.5}$ have a statistically significant positive linear correlation. However, turbidity on its own can prove insufficient in predicting PM2.5 value due to several aerosol characteristics affecting both the predictor and response variable. A new model is created by combining turbidity and meteorological conditions in order to estimate $PM_{2.5}$. We will present our theoretical approach and the details of our prediction capabilities of $PM_{2.5}$ in our presentation.

14LC.2

Airbox: A Participatory Ecosystem for pm2.5 Monitoring. LING-JYH CHEN, Shih-Chun Lung, Sachit Mahajan, Hsin-Hung Hsieh, Jin-Wei Liu, *Academia Sinica*

With emerging concerns of air pollution and recent advances in low-cost sensors, air quality monitoring has become one of the most important Internet of Things (IoT) applications in many countries and major cities. One of the most successful systems of this kind is the AirBox project, which is based in Taiwan and operated in a grassroot fashion, and it has deployment more than 4,000 nodes in more than 30 countries till now. The system is also notable for its extremely high deployment density and data frequency, as most of the participating nodes are located in Taiwan and with a high sample rate. In this work, we present the development of this AirBox project in detail, and we demonstrate several data analysis work that we have carried out for data visualization, anomaly detection, data forecast, and other advanced data services. We also discuss challenges and opportunities for making sense of Internet of Things data based on the lessons learned from the AirBox project.

14LC.3

Evaluation of a Low-Cost Personal Sampler for Assessing Respirable Dust Exposure in Taconite Mining. REBECCA FOOS, Nima Afshar-Mohajer, Karl Braun, Gurumurthy Ramachandran, John Volckens, *Colorado State University*

There have been significant advances in low-cost technologies for air sampling in recent years. Among the samplers currently being introduced to the market is the Ultrasonic Personal Aerosol Sampler, or UPAS (Volckens et. al. 2017). Several inlets have been developed for the UPAS to sample the fine particulate matter (PM2.5), inhalable particulate matter, and now the respirable fraction. A rigorous test of UPAS fitted with the respirable cyclone inlet in the field was lacking.

A taconite mining facility was selected as a suitable test location for evaluation of the respirable sampler performance. Beyond crude-ore extraction, taconite ore processing involves multiple stages of crushing, refining, and pelletizing to render a kiln-fired iron pellet ready for manufacturing. Each stage is characterized by unique aerosol profiles due to varied application of mechanical force and variable levels of water within the product. Representative employees from each production area volunteered to carry out personal collocations of the UPAS sampler with respirable cyclone and a traditional sampling pump with aluminum respirable cyclone. Participation requirements were limited to shift length alone, and partial shifts of fewer than eight hours were not sampled.

One hundred employees participated in the collocated deployment over the course of eight days. Pre-weighed filters were loaded into the respective UPAS cartridges and three-piece cyclone cassettes, and the UPAS and aluminum cyclone inlets were mounted in close proximity within the breathing zone of each participant and at the designed flow rates of 2.0 and 2.5 liters per minute respectively. Sampling duration varied between seven and twelve hours per the length of the employee shift. Following the field deployment, all filters were weighed again to determine the loaded filter weight.

Of the one hundred collocations, six were removed from the resulting data set due sampling error such as pump malfunction. The remaining ninety-four sets of filters were incorporated into the analysis. Total respirable mass was considered the primary metric. Adjusted for total volume sampled, the UPAS and traditional respirable samplers showed good agreement for total respirable particulate. Additional speciated analysis for various metallic elements as well as respirable crystalline silica is ongoing.

In conclusion, the occupational environment proved to be suitably rigorous, as demonstrated by the maximum filter loading and occupational exposure measured by the deployment. In such a heavy industrial setting, the Ultrasonic Personal Aerosol Sampler performed comparably to the traditional sampling train when sampling for the respirable fraction.

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14LC.4

A Novel Method Based on Light Scattering for Distinguishing Water and Fly-ash Aerosols in Industrial Stack Emission.

Satyanarayanan Seshadri, VIPUL DOGRA, *Indian Institute of Technology, Madras*

Light scattering experiments were performed to understand the difference in behaviour between water and fly-ash aerosols. Our intent is to differentiate liquid droplets from fly-ash found in industrial stack emissions, where liquid carry over is observed when flue gas de-sulphurization is used.

Qualitative differences in measuring spherical (poly styrene latex) and non spherical (talc) were presented using sphericity index as a measure has been proposed and used by [Sachweh, Dick and McMurry,2007]. Their studies were performed in a spherical flow through chamber instrumented with detectors on azimuthal and polar angles. In this study we found that polarization of incident light was altered by both water droplets and fly ash. However at certain polarization angles (φ_p) no scattered light from fly-ash was observed at the detector, while being present for water droplets.

Experiments were performed using fly-ash, mean particle diameter (d_p) = 24 µm, collected from biomass combustion exhaust. Fly-ash aerosols, generated using a turntable dust generator, was seeded into a vertical tunnel, where a mean velocity of 8 m/s was maintained. Water droplets with mean droplet size of 15 µm were generated from a pressure jet atomizer. A 532 nm light source was used to illuminate the flow with polarization applied at the source and detector side. Tests were conducted with fly-ash and water droplets alternatively.

Measurements performed at 10 degrees forward scattering angle revealed that the ratio of scattering signatures between ash and water droplets were 5 times lower with change in polarisation settings perpendicular to plane of scattering as compared to in-plane polarisation. Preliminary studies reveal statistically significant differences, enabling quantitative assessment of ratio of water to dust particles in a mixed flow system. Results are compared to standard gravimentric sampling.

Industrial emission stacks currently suffer from over reporting of particulate emission data due to errors from moisture. Liquid carry over can be as high as 6%, confounding traditional CEMS (continuous emission monitoring systems) involving triboelectric or light extintion based measurement systems. With this development, we could propose design of an instrument that could in-situ correct for errors from counting water droplet, thereby reducing false alarms.

14LC.5

Intelligent PM2.5 Sensor Network Experience in Taiwan's Campus and Industrial Park. HSUNLING BAI, Chungsying Lu, Shie-Yuan Wang, Wen-Chih Peng, Chun-Chia Hsu, Sihyu Liou, Chienchiao Hung, Yen-Chi Huang, Peiyu Lu, Wei So Sun, *National Chiao Tung University*

This study presents the collaborate work of a cross-domain research through environmental, cloud computing and big data analysis to create a new generation of air quality monitoring systems using low cost sensors. The intelligent sensing experience of ambient $PM_{2.5}$ monitoring in a university campus and an industrial park was reported. The Plantower PMS7003 $PM_{2.5}$ sensor (brief as "G7 sensor" hereafter) was selected in the intelligent sensor network because it outperformed other tested sensors in terms of precision and accuracy. After lab calibration, the G7 sensors were installed in the NCTU campus to construct a small $PM_{2.5}$ sensing network via the Internet of Thing (IoT) technology. A small cloud system that can store and provide $PM_{2.5}$ sensed data has also been built. The data loss rates during transmission were evaluated under different circumstances. And several data mining methodologies have been approached to simulate and predict the sensed data for the purposes of identifying outliers and pollution sources as well. Further field experience was then gained by building another intelligent sensing network in an industrial park. Field calibration of the $PM_{2.5}$ low cost sensors with the FEM instrumentation data obtained from nearby air quality monitoring stations was established. And the field calibration results were compared with the original lab calibration results.

14LC.6

Using Low-Cost Sensors (RAMPs) to Evaluate the Spatial and Temporal Variation of Fine Particulate Matter Concentration within Environmental Justice Communities Surrounding Large Industrial Facilities.

REBECCA TANZER, Carl Malings, Allen Robinson, R. Subramanian, Albert Presto, *Carnegie Mellon University*

The state-of-the-art in air quality monitoring consists of a sparse network of precise reference instruments which give limited information on the spatial distribution of pollutants. Thus, there is value in reliable low-cost air quality monitors that can be deployed in large numbers to more accurately assess spatial variation in pollutant concentrations. One specific use case is to evaluate environmental injustice near industrial point sources. We have developed low-cost air quality monitors called Real-time Affordable Multi-Pollutant (RAMP) sensor packages. The RAMPs include light scattering nephelometers for measurement of fine particulate matter ($PM_{2.5}$). A network of fifty RAMPs have been deployed throughout Pittsburgh, PA. A subset of nine RAMPs have been deployed within the Monongahela River Valley, an environmental justice region, with major industrial sources. The largest coke plant in the US located in Clairton and a steel mill in Braddock both contribute to the historic nonattainment of the Monongahela River Valley to National Ambient Air Quality Standards.

Nine RAMPs are currently deployed to capture a range of microenvironments near the point sources. Three RAMPs are west/southwest (typically upwind) of both the coke plant and steel mill. Three RAMPs are immediately downwind (within two miles) of the coke plant. The three remaining RAMPs are immediately downwind of the steel mill (within two miles). The distribution of RAMPs allows us to quantify changes in outdoor $PM_{2.5}$ concentrations in both space and time; comparison of source-impacted RAMPs to RAMPs located upwind and in the Pittsburgh urban core allow us to evaluate the local contribution of these point sources.

There is substantial spatial variation in times and durations of elevated $PM_{2.5}$ concentrations between test areas. $PM_{2.5}$ concentrations near the steel mill, downwind of the coke plant, and upwind of the coke plant are higher than 12ug/m^3 (the EPA annual average $PM_{2.5}$ standard) for 32%, 33%, and 22% of the deployment time, respectively. The percent of the time that the hourly averaged $PM_{2.5}$ concentration is above short-term (daily) standards set by the WHO (25ug/m^3) for the steel plant location, downwind of the coke plant, and upwind of the coke plant are 8%, 10.6%, and 3.5% respectively. Even though these locations are less than ten miles apart significant differences exist between their $PM_{2.5}$ concentrations.

The value of a distributed network of low-cost monitors is demonstrated by the fact that high concentration periods measured at one location are not always experienced at the other sites. For example, a period of over four hours measured concentrations above 60ug/m^3 at the location downwind of the coke plant while no such elevated concentration event was recorded at the other test locations during the same period of time. Periods of elevated $PM_{2.5}$ concentrations (incidents where the hourly averaged $PM_{2.5}$ concentration was over 25ug/m^3) lasting for over ten hours are more likely to occur downwind of the steel and coke plants than they are to occur upwind of the coke plant or in an urban Pittsburgh neighborhood. Further analysis will be conducted into assessing the $PM_{2.5}$ concentration at additional downwind locations to determine the change in $PM_{2.5}$ concentration over increasing distance from an industrial facility. Deployment of sensors at the original nine sites began in Spring 2017. Over a year's worth of data at multiple sites will enable the analysis of seasonal changes in pollutant spatial heterogeneity within these environmental justice regions.

14RA.1

Temporal Distribution of New Particle Formation Events in Brisbane, Australia. BUDDHI PUSHPAWELA, Rohan Jayaratne, Lidia Morawska, *Queensland University of Technology, Brisbane, Australia*

The formation of secondary particles in the atmosphere through homogeneous nucleation is known as new particle formation (NPF). This is one of the major sources of particles in the atmosphere and has been observed in different environments around the world including in urban, industrial, agricultural and coastal sites, as well as in boreal forests and the polar regions.

In this study, we collected data of charged and uncharged particle concentrations in the urban environment of Brisbane using a Neutral cluster and air ion spectrometer (NAIS) on nearly 500 days over three calendar years. The NAIS is able to measure particles down to their smallest size of 2 nm. The measurements were carried out at the Gardens Point Campus of the Queensland University of Technology in Brisbane, Australia. The main sources of atmospheric pollution at this site are motor vehicle exhaust emissions, emissions from the Brisbane port and oil refineries.

We identified NPF events using the rate of change of total particle concentration, dN/dt, where N is the number of particles in the size range 2.0 -10.0 nm. Events with N > 10,000 cm^{-3} for at least 1 hour and dN/dt >10,000 cm^{-3} h^{-1} were defined as “strong” NPF events. Events with 5000 < N < 10,000 cm^{-3} for at least 1 hour and 5000 < dN/dt < 10,000 cm^{-3} h^{-1} were classified as “weak” NPF events. These events generally exhibit a “banana” shape in the contour plot of particle number concentration (PNC) vs time.

Every NPF event was characterised by a sharp increase of the PNC in the intermediate size range from 2.0-7.0 nm. In this study, the starting time of a strong NPF event was determined by noting the time of first occurrence of dN/dt > 10,000 cm^{-3}h^{-1}, where N is the number of particles in the size range 2.0-10 nm. The starting time of a weak NPF event was determined by noting the time of first occurrence of dN/dt > 5000 cm^{-3}h^{-1}.

During the three-year period of monitoring, we acquired 485 complete days of data and observed 177 strong NPF events (an occurrence rate of 37%). We also observed 59 weak NPF events (an occurrence rate of 12%). These high occurrence rates suggest a possible link between NPF and high concentrations of gaseous precursors from motor vehicles and industry in the urban environment of Brisbane. Seasonal dependency on NPF showed that the probability of occurrence of NPF was highest during the summer (43.8% in November-February) and lowest during the winter (32.1% in May-August). However, the difference in mean temperature in Brisbane between summer and winter is not as great as in more temperate climates.

Further, we derived the first diurnal variation chart of NPF events anywhere in the world. We found that 74% of NPF events began during the morning, with a high likelihood occurrence between 8:00 and 8:30 am. This starting time coincides very well with the morning rush hour traffic when the production rate of gaseous precursors is generally at a maximum.

Another important observation from this study was that the NPF starting times were not dependent on season. There is a two-hour time difference in sunrise between winter and summer in Brisbane. Therefore, we conclude that NPF events in Brisbane are driven more by traffic density rather than by solar radiation intensity.

14RA.2

New Particle Formation and Sub-10nm Size Distribution Measurements in Paphos, Cyprus, during the A-LIFE Field Experiment. SOPHIA BRILKE, Nikolaus Fölker, Konrad Kandler, Nan Ma, Thomas Müller, Anne Philipp, Thomas Ryerson, Petra Seibert, Bernadett Weinzierl, Paul M. Winkler, *University of Vienna*

Atmospheric new particle formation (NPF) is a frequent phenomenon that is significantly contributing to the global aerosol budget throughout the troposphere. Newly formed particles can affect human health and potentially grow to sizes large enough to influence the Earth's radiation balance and climate.

In this study, we aim at characterizing NPF and early nanoparticle growth in the Eastern Mediterranean region during the ERC-funded A-LIFE (**A**bsorbing aerosol layers in a changing climate: aging, **LIFE**time and dynamics) field experiment. The A-LIFE intensive measurement campaign in April 2017 combined in-situ and remote sensing measurement techniques both at the ground and on the Deutsches Zentrum für Luft- und Raumfahrt (DLR) research aircraft Falcon. The overall aim of A-LIFE is to study the properties of absorbing aerosols (i.e. mineral dust – black carbon mixtures) and investigate potential links between the presence of absorbing particles, aerosol layer lifetime and removal.

The understanding of the processes leading to NPF requires particle measurements down to the critical size of freshly formed particles. Sub-10nm particle size distribution measurements are extremely challenging due to high diffusional loss rates in the sampling and measurement system. Novel measurement techniques enable the detection of newly formed particles at a decent sensitivity: the DMA-train, designed for sub-10nm size distribution and precise growth rate measurements, was first set up in an atmospheric experiment. The DMA-train setup consists of six Differential Mobility Analysers (DMA) operated in parallel followed by condensation particle counters (CPCs) tuned for the detection of the smallest particle sizes at a time resolution of 1s with the lowest channel set at 1.8nm. The Scanning Mobility Particle Sizer (SMPS) scanned the size distribution onwards between 10 and 800nm in 5min intervals whereas the total particle concentration was obtained from a Particle Size Magnifier (PSM) - CPC combination every second.

During the 30-day measurement period at the coastal ground-based station in Paphos (Cyprus), we observed 9 NPF events during morning hours and were able to follow the initial particle growth in the DMA-train. In 5 cases, however, the initial growth was interrupted below 10nm and only 4 growth events were detected by the SMPS. This finding suggests that NPF may happen much more frequently than is currently thought but is oftentimes not captured well enough by regular SMPS. The local wind pattern is dominated by a land-sea-breeze system with NE and NW being the prevailing wind directions. The typical diurnal picture reveals highest total particle concentrations together with elevated NO/NO_2 and SO_2 concentrations for air masses carried to the station from the interior of the island during night hours. NPF events were found during both NE and NW wind situations. Furthermore, we use the FLEXPART (**FLEX**ible **PART**icle dispersion model) model in order to better understand on a large scale the origin of air masses that favour NPF.

In our presentation, we present results from the A-LIFE field experiment with the special focus on the parameters influencing NPF and initial particle growth in Cyprus. We will include size distribution data obtained by the DMA-train and correlations between particle and trace gas data as well as meteorological parameters. In addition, the backward trajectory analysis from FLEXPART and possible implications on NPF will be discussed.

14RA.3

Identification of New Particle Formation Events with Deep Learning. Jorma Joutsensaari, MATTHEW OZON, Tuomo Nieminen, Santtu Mikkonen, Timo Lähivaara, Stefano Decesari, M. Cristina Facchini, Ari Laaksonen, Kari Lehtinen, *University of Eastern Finland*

New particle formation (NPF) in the atmosphere is observed frequently in different environments in the boundary layer. It has been estimated that 30–50% of global tropospheric cloud condensation nuclei concentrations might be formed by NPF. Currently, NPF events are typically classified into different event classes manually from the measurement data by researchers. This is time consuming and the identification of event type might be inconsistent. To get more reliable and consistent results, the NPF event analysis should be automatized.

We have developed a novel deep learning-based method to identify automatically NPF events (Joutsensaari et al., 2018). The method is based on image recognition of daily-measured particle size distribution data. In image analysis, we utilized a commonly available pre-trained Convolutional Neural Network (CNN), named AlexNet, which was transfer learned to recognize NPF event classes (six different types). In transfer learning, a subset of particle size distribution images were used in the training stage of the CNN and the rest of images for testing the success of the training. The event classification was done directly from existing data (figures) without any pre-processing of the data. To our knowledge, this is the first time when an automatic method has been successfully used to classified NPF event into different classes.

We utilized the developed method for a 15-year long dataset measured at San Pietro Capofiume in Italy. The results showed that clear event (i.e., even types of Classes 1 and 2) and non-event days could be identified with an accuracy of ca. 80 %, when the CNN-based classification was compared with visual-based classification by researchers. In the event analysis, the choice between different event classes could be ambiguous and thus overlapping between different classes occurs easily. The results showed that the overlapping occurs typically between the adjacent event classes, e.g., a manually classified Class 1 was categorized into Classes 1 and 2 by CNN, etc. In general, the manual and CNN classifications were very consist for most of the days. Clear misclassifications seemed to occur more commonly in manual analysis than in the CNN categorization, mainly due to a wrong or an incorrectly listed classification by researchers.

In general, the automatic CNN-based classification seems to have a better reliability and repeatability in NPF event classification than human-made visual-based classification. Typically, an analysis of large long-term datasets requires manual labor of several researchers, which is very time consuming and the quality of the analysis may vary. Therefore, the transfer learned pre-trained CNNs are powerful tools to analyze any long-term datasets more accurately and consistently in a sufficiently short time, which helps us to understand in detail aerosol-climate interactions and the long-term effects of climate change on NPF in the atmosphere.

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14RA.4

Long-term Trends in Particle Number Size-distributions and New Particle Formation Observed at San Pietro Capofiume, Italy.

TUOMO NIEMINEN, Jorma Joutsensaari, Ville Leinonen, Santtu Mikkonen, Taina Yli-Juuti, Pasi Miettinen, Annele Virtanen, Kari Lehtinen, Ari Laaksonen, Stefano Decesari, Leone Tarozzi, M. Cristina Facchini,
University of Eastern Finland

Atmospheric aerosols have a large impact on air quality, human health and even the global climate. Both the aerosol number concentration and their size have influence on the climatic effects of aerosols. Formation and growth of secondary aerosol particles is a major source of atmospheric aerosols, and has been a subject of active research during the past two decades. However, only few long-term datasets (over 10 years of measurements) of atmospheric aerosol number size distributions exist[1,2,3,4].

In this work, we characterize trends in aerosol number size-distributions and in new particle formation (NPF) at San Pietro Capofiume in Po Valley, Northern Italy. Number size distributions of 3–630 nm particles have been measured there continuously since March 2002 with a twin-DMPS setup. The site is influenced by emissions of local anthropogenic pollutants (such as SO_2) as well as long-range transport from Central and Eastern Europe, and thus can provide information on the impact of anthropogenic activity on aerosol size-distributions and NPF.

The particle number size-distribution data was classified into NPF event, non-event and undefined days[5]. The formation and growth rates of nucleation mode particles (defined here as particles of 3–25 nm in diameter) were calculated based on the time-evolution of the measured number size-distribution data. To quantify the trends in particle concentrations, we have used two methods. The first method fits the concentration time series as a sum of constant linear trend and seasonally varying component. The statistical significance of the fitted trend is estimated by performing the fitting multiple times with bootstrap sampling. The second method is a Dynamic Linear Model (DLM)[6], where the particle number concentration timeseries is decomposed into level, trend, seasonality, and noise. These components are allowed to change as functions of time, and the magnitude of this change is modelled and estimated[7].

There has been a longer break in the measurements from November 2010 until June 2011, during which time the twin-DMPS setup was in maintenance. Before this break, statistically significant decreasing linear trends are observed in nucleation, Aitken and accumulation mode particle concentrations. The largest decrease (–10%/year) occurs in the nucleation mode particle concentration. After the measurement break, only the nucleation mode particle concentration shows a statistically significant trend (decreasing –4.9%/year). The DLM method indicates that these changes occurred in 2008–2009. The particulate mass concentrations (PM_{10} and $PM_{2.5}$) have also been reported to decrease throughout the Po Valley region, and it is attributed to decreases both in primary emissions and in precursors of secondary inorganic aerosol emissions mostly from vehicular traffic[8]. However, unlike the change in the trends of the particle number concentrations after 2007–2008 seen in our study, the PM concentrations seem to have continued their decrease until at least 2014.

The annual frequency of NPF event occurrence did not show any clear trend, varying between 20% and 40% of the days in a year. Both the formation and growth rates of nucleation mode particles had a decreasing trend of –3%/year and –2%/year, respectively. This would indicate that even though the sink for the newly formed particles has decreased (due to decrease in PM concentrations), a simultaneous decrease in precursor vapour emissions (sulphur dioxide, ammonia, amines, organics) has also occurred.

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14RA.5

Measuring Light Absorption by Organic Aerosols: Correction Factors for Solvent Extraction Based Photometry Techniques. NISHIT SHETTY, Apoorva Pandey, Wei Min Hao, Rajan K. Chakrabarty, *Washington University in St. Louis*

Recent studies have shown that organic carbon (OC) aerosol could have a non-trivial role in atmospheric light absorption at shorter visible wavelengths. Good estimates of OC absorption are therefore necessary to accurately calculate radiative forcing due to these aerosols in climate models. One of the common techniques used to measure OC light absorption is the solvent extraction technique from filter samples which involves the use of a spectrophotometer to measure the bulk absorbance of the solvent-soluble organic fraction of particulate matter. The bulk absorbance is subsequently converted to particulate absorption using correction factors. The appropriate correction factors to use for performing this conversion under varying scenarios of EC/OC ratios has been an unexplored area of research. The conventional view is to apply a correction factor of 2 for water-extracted OC based on Mie calculations.

We performed a comprehensive laboratory study involving four solvents (water, methanol, acetone, hexane) to investigate the corrections factors for primary OC aerosol emitted from biomass burning as a function of EC-to-OC ratio and single scattering albedo (SSA). The aerosol emissions were collected on quartz fiber filters for calculating their bulk OC absorption coefficients using UV-Vis spectrophotometry. In parallel to the filter sampling set up, the aerosols were simultaneously measured for their particle-phase optical properties using multi-wavelength integrated photoacoustic nephelometers. Conversion factors for bulk-to-particulate OC absorption were calculated. Additionally, from the spectroscopic data, we analyzed and compared the Absorption Ångstrom Exponents derived from both analytical techniques. This presentation will conclude with recommendations for future research needed in this direction.

14RA.6

Aerial Observation of Atmospheric Nanoparticles in Fukue Island, Japan. KWANGYUL LEE, Indra Chandra, Yayoi Inomata, Yoshio Otani, Masahiko Hayashi, Akinori Takami, Takafumi Seto, *Kanazawa University*

Nucleation and new particle formation (NPF) in the East Asia region is strongly influenced by the photochemical processes during long range and trans-boundary transport of air pollutants. Our previous measurements (Seto et al., 2013; Indra et al., 2016) related with the incomplete and weak NPF (starting from ~10 nm) at Fukue island (downstream) are suggesting the nucleation in upstream flow. Aerial observation has great advantages for the investigating nucleation and NPF over certain region. Vertical structure of atmospheric nanoparticle concentration (particle size >6 nm and altitude 1), and air mass backward trajectory analysis. The stronger NPF event (Event I, >35,000 cm^{-3}) than our previous measurements (from 2012 to 2016, ~20,000 cm^{-3}) with the particle size as small as 5 nm affected by the long range transport of air pollutants under a high pressure system was detected. In addition, sudden increase of particle number concentration and SO_2 concentration with weak NPF (onset diameter above than 10 nm) caused by the change of air mass origin (Event II, <10,000 cm^{-3}) and no NPF with aged sulfate particles under low particle number concentration and low SO_2 condition (-3) were observed. Vertical profile and size distribution of nanoparticles, meteorological condition, chemical composition of submicron (< 1 µm) particles, SO_2 concentration and air mass backward trajectory based on different events were analyzed.

14SA.1

Going Deeper on the Characterization of the Biogenic SOA by Combining On-line and Off-line Approaches during F-BEACh 2014. LAURENT POULAIN, Anke Mutzel, Monique Teich, Nadja Triesch, Andreas Held, Stefanie Richters, Dominik van Pinxteren, Yoshiteru Iinuma, Martin Brüggemann, Alfred Wiedensohler, Hartmut Herrmann, *Leibniz Institute for Tropospheric Research*

Secondary Organic Aerosol (SOA) is resulting from reactions of Volatile Organic Compounds (VOCs) emitted into the atmosphere either from anthropogenic or biogenic sources. Although SOA represents an important fraction of the total organic aerosols mass, up to now models mostly underestimate the ambient SOA concentrations, indicating that some of the SOA formation mechanisms and/or sources are still not well characterized or missing. One of the dominant SOA sources is related to biogenic emissions from plants and trees.

In order to better assess biogenic SOA, an intensive field campaign took place at the forest research station of the University of Bayreuth (Germany) in July 2014 (Fichtelgebirge – Biogenic Emission and Aerosol Chemistry, F-BEACh 2014). A complementary set of real time mass spectrometers, including a High Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS), a Chemical Ionization Atmospheric-Pressure interface Time-of-Flight Mass Spectrometer (CI-APiToF-MS) and an Aerosol Flowing Atmospheric-Pressure Afterglow Mass Spectrometer (AeroFAPA-MS), was deployed. Additionally, off-line analysis on day-night regime of High-Volume filter samples (Digitel PM_1) performed in parallel was made and targeted to biogenic SOA tracers (*e.g.*, monoterpene tracers, organosulfate and nitroxyorganosulfate compounds), carboxylic acids, carbonyls, imidazoles, amines and amino-acids as well as highly oxidized multifunctional organic compounds (HOMs) tracers.

Source apportionment was performed using Positive Matrix Factorization (PMF) based on the high-resolution AMS mass spectra. In contrast to the traditional PMF approach, inorganic fragments were added to the organics mass spectra matrix, in order to distinguish inorganic and organic sulfate and nitrate compounds, and therefore, investigate the complete non-refractory near PM_1 (NR-PM_1) particle composition measured by the AMS. Validation of the PMF results was made by comparison with off-line results. It was therefore possible to clearly distinguish two groups of factors: one associated to long-range transport/regional background (three different factors representing approx. 44% of the NR-PM_1 mass) and several local SOA factors. From the last group, it was possible to distinguish a nitrate related organic aerosol associated to semi-volatile compounds, an organo-nitrate related factor, a freshly locally formed monoterpene SOA factor, a non-monoterpene SOA factor and a possible primary biogenic organic aerosol factor (all together 56% of the NR-PM_1). Details on the source apportionment results and factors identification will be presented.

14SA.2

Chemical Characterization and Source Contribution to PM2.5 Organic Fraction in Neighboring Towns of Bogota, Colombia. Felipe Villamil, Irene Rosas, James Schauer, NESTOR ROJAS, *Universidad Nacional de Colombia*

Fast urbanization processes have occurred in Latin America in the last four decades, making it the region with the highest urbanization rate in the world, with more than 80% of its population living in cities. Unfortunately, rapid growth has not been accompanied by long-term urban planning strategies or robust environmental controls. As a result, and despite improvements made in the last decade, cities in the region have traditionally had an obsolete vehicle fleet and highly polluting industries within densely populated areas. Recent economic growth has worsened the problem by sharply increasing motorization rates as a consequence of higher income per capita and, hence, intensifying traffic congestion and emissions. Small towns and cities within large metropolitan areas or close to larger cities in the region are now following similar processes and some of them have already suffered the impacts of these dynamics.

Air quality in Bogota's neighboring towns is affected by their own emissions and by pollution transported from this city of more than 8 million inhabitants. However, little is known about the characteristics and sources of pollutants affecting their population. The Sabana Occidente county, with ca. 420,000 inhabitants, and the Soacha county, with ca. 550,000 inhabitants, are of special interest because of the presence of important industrial corridors in the towns of Soacha, Mosquera, Funza, Madrid and Facatativa; mining of construction materials and clay in Soacha; and national roads that connect Bogotá with western and southern cities and the Pacific coast. This work focuses on these counties, with sites in Soacha and Mosquera, where we investigated the contribution of different types of sources to PM2.5. We collected 24-h PM2.5 samples for a two-month period at each site and analyzed them for mass, elemental and organic carbon, water-soluble organic carbon and inorganic ions. We analyzed two- and three-day composites for particle-bond organic tracers. Then we used EPA's Chemical Mass Balance (CMB) receptor model to determine the source contributions to the particulate organic fraction. Average PM2.5 mass concentrations were similar for Soacha (31 ug/m3) and Mosquera (26 ug/m3). Organic matter was the major component of PM2.5 for all sites, constituting 68% of the PM2.5 mass in Soacha and 63% in Mosquera. We identified 5 sources of the particulate organic fraction at both sites: wood smoke, diesel vehicles, gasoline vehicles, natural gas combustion and industrial coal combustion. However, the contribution differed between sites. Wood smoke was the predominant source in Soacha, accounting for 40% of the organic fraction, followed by gasoline vehicles (18%), diesel vehicles (13%), industrial coal burning (2%) and natural gas burning (1). A quarter of the organic fraction (26%) is contributed by still unidentified sources. In Mosquera, diesel and gasoline vehicles have a similar contribution (18%), followed by wood smoke (10%), industrial coal burning (7%) and natural gas burning (1%). A very significant fraction of organic matter (46%) is contributed by still unidentified sources. Secondary inorganic ions (ammonium, sulfate and nitrate) constitute about 10% of the PM2.5 mass.

14SA.3

Comprehensive Analysis of PM2.5 in Toronto: Composition, Sources, and Health Effects. CHEOL H. JEONG, Alison Traub, Angela Huang, Jon M. Wang, Nathan Hilker, Anthony Munoz, Ewa Dabek-Zlotorzynska, Dennis Herod, Scott Weichenthal, Greg J. Evans, *SOCAAR, University of Toronto*

In order to provide a historical perspective of fine particulate matter (PM2.5), source apportionment was conducted on 13-year comprehensive aerosol chemical speciation data collected from 2004 to 2016 in downtown Toronto, Canada using a Positive Matrix Factorization (PMF). The PM2.5 samples were collected every three days using two 24-hr integrated filter samplers operated by Environment and Climate Change Canada to measure PM2.5 mass, inorganic ions, thermal/optical organic carbon (OC) and elemental carbon (EC), and trace elements. In addition to the integrated samples, hourly-based continuous particulate measurements for inorganic and organic aerosol, trace metals, OC, EC, and optical black carbon were conducted at the downtown site since 2011. The objective of this study was to compare the 24-hr integrated filter data to the hourly-resolved chemical speciation data, to identify the long-term trend of PM2.5 sources in the urban area, and to evaluate the PMF analysis using these PM2.5 speciation data. Furthermore, the oxidative potential (OP) of PM2.5 samples was also determined to investigate the influence of PM2.5 trace elements on the capacity of PM2.5 to generate reactive oxygen species. To assess the temporal and spatial variability of the OP of PM2.5, we examined the oxidative potential of PM2.5 samples collected over a year-long period at three sites, downtown, urban background, and highway. The PMF-resolved sources were compared to the OP to identify PM2.5 sources affecting the temporal and spatial distribution of aerosol oxidative potential. The results will provide insight into the associations between source impacts and OP for both air quality policy decisions and heath studies.

14SA.4

Source Apportionment, Wind Transport and Atmospheric Transformation of Carbonaceous Aerosol in the San Joaquin Valley, California. BENJAMIN DE FOY, Michael Olson, Alexandra Lai, Min-Suk Bae, Qingyang Liu, Matthew Skiles, James Schauer, *St. Louis University*

PM2.5 samples were collected in Fresno and Bakersfield, California, from Jan 2015 to Feb 2016. The samples were collected over 24 hours every third day, matching the samples from the Environmental Protection Agency's Chemical Speciation Network (EPA CSN). Chemical Mass Balance (CMB) and Positive Matrix Factorization (PMF) were applied to the chemical composition of the samples to obtain estimates of major sources contributions to ambient carbonaceous aerosols. There was a strong seasonality in the contributions of some sources as well as dependence on wind transport. Meteorological analysis of surface winds and radar wind profiler data was applied to distinguish the impact of source variations, chemistry and wind transport on the sample concentrations. Back-trajectories using WRF-FLEXPART were used to further characterize wind transport and residence times in the Central Valley. Clustering of the trajectories revealed dominant wind patterns and were combined in a multiple linear regression model to identify source regions. The meteorological analysis further revealed the importance of stable atmospheric conditions in the valley and the impact of the "Fresno Eddy" in contributing to air quality exceedances. The results from the fourteen-month study were compared with long term trends based on measurements of criteria pollutants from the Air Quality System (AQS). These were available at multiple sites in the valley at an hourly resolution, which provided a database with hundreds of thousands of data points. Analysis of these time series was used to estimate the trends in emissions on an annual, seasonal, weekly and diurnal timescale. The AQS data also provided constraints on the impact of transport and meteorology on high pollution events and air quality exceedances. By combining the analysis of speciated aerosol measurements with long time series of criteria pollutants, the analysis identified improvements in air quality over the last decade and avenues for future improvements.

14SA.5

Ambient PM2.5 Source Apportionment: a Case Study of Tehran. SINA TAGHVAEE, Mohammad Sowlat, Amirhosein Mousavi, Mohammad Sadegh Hassanvand, Masud Yunesian, Kazem Naddafi, Constantinos Sioutas, *University of Southern California*

In this study, $PM_{2.5}$ source apportionment is performed using Positive matrix factorization (PMF) for two sampling site in the central part of Tehran (i.e."Tohid retirement home" and "school dormitory") to identify the main contributing sources to $PM_{2.5}$ mass concentration. To achieve such goal, $PM_{2.5}$ mass, water-soluble ions, and metals concentrations were used along with other auxiliary variables such as elemental and organic carbon (EC/OC), and meteorological data for identification and quantification of $PM_{2.5}$ sources. A 7-factor solution was selected as the most acceptable and plausible one for both locations based on the evaluation of the resulting source profiles, temporal trends of each factor in cold phase (i.e. fall and winter) and warm phase (i.e. spring and summer), correlation analysis between EC/OC data and PMF resolved factor contributions, analysis of bootstrap runs, and R^2 values of predicted vs. measured $PM_{2.5}$ concentration . The factors included vehicular emissions, secondary aerosol, industrial emissions (i.e. industrial emissions 1 and 2), biomass burning, soil, and road dust in "Tohid retirement home". On the other hand, vehicular emissions, secondary aerosol, industrial emissions, biomass burning, soil, brake wear particles, and tire dust were the 7 factors resolved by PMF for another sampling site. Results indicate that most of the contribution belongs to vehicular emissions, with slightly higher contribution in "School dormitory" (49.3%) compared to "Tohid retirement home" (48.8%). Secondary aerosol has also the second highest percentage of contribution in both locations, with higher contribution in "Tohid retirement home" rather than "school dormitory" which might be reasonable due to its more distance from major traffic flows. In addition, while two industrial factors were identified in "Tohid retirement home" (with totally more than 17% contribution), only one industrial factor (less than 2 % contribution) is recognized in another sampling site which might be due to the fact that the retirement home is more impacted by industrial activities. The other resolved factor profiles for "Tohid retirement home" were biomass burning, soil, and road dust with relative contributions of 3%, 2.8% and less than 1% respectively. Biomass burning, soil, and the remaining non-tailpipe road emissions (including brake wear particle and tire dust) were also accounting for 16%, 8.2%, and less than 1% of total $PM_{2.5}$ mass concentration in "school dormitory". Results of this study can be used as a beneficial tool for policy making purposes regarding air quality improvement and addressing adverse health effects of $PM_{2.5}$.

14SA.6

Comparison of PM2.5 Chemical Composition and Sources at a Rural Background Site in Central Europe between the Years 1993/1994/1995 and 2009/2010: Effect of Legislative Regulations and Economic Grow on the Air Quality. PETRA POKORNÁ, Jaroslav Schwarz, Radek Krejci, Erik Swietlicki, Vladimír Havránek, Vladimír Ždímal, *Institute of Chemical Process Fundamentals CAS*

In this work, the $PM_{2.5}$ chemical composition data from the first half of the 1990s, thus 5 years after the switch-over from Communist rule in Czech Republic, enable to assess the influence of legislative regulations and economic grow on the air quality within the period of 15 years. The objective of this study is to compare the $PM_{2.5}$ chemical composition and sources at a rural background site in Central Europe between the years 1993/1994/1995 and 2009/2010.
From December 1993 to January 1995 and from October 2009 to October 2010, a total of 320 and 365 daily samples of the $PM_{2.5}$ were collected at a rural background site (National Atmospheric Observatory Košetice) in Central Europe. Chemical analysis of $PM_{2.5}$ for 29/26 elements by PIXE and water-soluble inorganic ions by IC (2009/2010) was performed. The Positive Matrix Factorization (PMF) was applied to the chemical composition of PM2.5 to identify its sources. The results of chemical analysis and source apportionment have been compared. The decrease of almost all elements concentrations, especially the metals regulated by the EU Directive, are evident. The median ratios show significant improvement in levels of analysed elements in $PM_{2.5}$. Slight increase of K levels and rs 0.09 K/Se points to rise in the residential wood combustion. The S levels are nearly comparable (higher mean in 2009/2010, while median ratio under 1). Change in the seasonal trends for K, Zn, Pb, Cu and partially S reflect change in dominating pollution sources of these elements. The apportioned sources in the years 1993/94/95 were brown coal combustion, oil combustion, sea salt and dust – long-range transport, re-suspended dust and black coal combustion. The industrial combustion of brown and/or black coal (rs 0.75 Se/As, rs 0.57 Ga/Ge and rs 0.20 As/Zn) and oil (rs 0.72 V/Ni) of the regional origin dominated. In the years 1993/1994/1995 the potential source regions were Czech-German-Polish border (brown coal), Moravia-Silesia region at the Czech-Polish border (black coal), and Austria, Hungary, Slovakia and Balkan (oil). The six factors in the years 2009/2010 were assigned as sulphate, residential heating, nitrate, industry, re-suspended dust, and sea salt and dust – long-range transport. The secondary sulphate from coal combustion and residential biomass burning (r_s 0.96, K/K^+) of the local origin dominated.
The declining trend of the elemental concentration and share of the $PM_{2.5}$ sources within the 15 years confirmed positive impact of the legislative regulations and economic grow.

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