

Plenary I: Friedlander Lecture

Airborne Ultrafine Particles and Nanomaterials: Adverse Effects on the Respiratory System and Beyond. FLEMMING R. CASSEE, *Dutch National Institute for Public Health and the Environment*

The adverse effects of air pollution on respiratory and cardiovascular health have been established in a series of major observational studies. Even short term exposures to particulate matter (PM) pollution have been associated with marked increases in cardiovascular morbidity and deaths from myocardial ischemia, arrhythmia and heart failure. However, these observational data are limited by imprecision in the measurement of pollution exposure, and the potential for environmental and social factors to confound these apparent associations. Much attention has been paid to the role of tail pipe emissions on pulmonary and cardiovascular toxicity. Examples will be shown on the implications of particles traps, catalytic converters and changing fuels (biodiesel) on the toxicity and health risk associated with tailpipe emissions. Although the focus in the past few years has been on road traffic emissions, mainly from diesel engine, PM is emitted from other sources like brakes as well as well as e.g. aviation. Some sources have been shown to have a much higher oxidative potential compared to diesel soot. This will also include BioPM, a suspension of particles containing living microorganisms or parts thereof released in air. Very little is known as to what extent such effects are different for PM obtained from other sources. Similarities and differences with engineered nanomaterials will be discussed. For a causal association to have scientific credence, a clear mechanism must be defined. Oxidative stress has been suggested as a key aspect leading to cardiovascular toxicity and worsening of diseases. This presentation will provide information on the effects of inhaled ultrafine particles and nanomaterials (including the role of physical and chemical properties) on the respiratory system as well as on cardiovascular health, neurodegeneration and reproduction.

Plenary II

What to Do About the Toll Biomass Burning is Taking on our Health, Indoor Environments, and Climate. SHELLY MILLER, *University of Colorado Boulder*

Biomass burning emissions include those from wildfires, controlled and agricultural burns, and burning of biofuels for heating and cooking. Emissions of aerosols and gaseous pollutants from burning biomass have major impacts on air quality, public health, and climate at spatial scales that range from indoors to global. Impacts are felt in developed and developing countries alike. Exposures are experienced mostly indoors due to the time we spend at home, so the focus of this presentation will be on indoor-related impacts. Particulate matter is of special interest because of the large quantity produced during biomass combustion and because of its known adverse human health outcomes, including increased hospitalizations, mortality, respiratory symptoms and infections, and inflammation. Climate change is increasing the frequency of wildfires and area burned; also, biomass burning is linked to changing the climate. This presentation will detail the latest science on impacts of biomass burning on indoor environments including wildfire impacts on residential exposure and biofuels combustion in homes in developing countries. Additional comments will include indoor cooking emissions from food preparation because this is a significant source of exposure to aerosols and toxic gases. A discussion of what can we do about it includes control strategies to effectively reduce exposures with ventilation, window opening, air cleaners, alternative fuels, and cleaner stove technology.

Plenary III**Soot Formation and Chemical Evolution during Combustion.**HOPE MICHELSEN, *University of Colorado Boulder*

There are substantial gaps in our understanding of the mechanisms controlling soot inception, particle growth, 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. These complexes are known as “incipient particles”, and the search for their formation and growth mechanisms is a subject of active research [1-3]. These incipient particles undergo further particle growth, generating liquid-like hydrocarbon particles, which eventually reach sizes in the range of 10-50 nm, known as “primary particles” [1-5]. 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 [4,5]. At high temperatures in the presence of oxygen, the aggregates fragment [6,7], and the primary-particle sizes and volume fractions decrease through oxidation [4,8]. There is a poor understanding of the mechanisms by which particles undergo these transitions and the parameters that influence them.

This talk will describe our current understanding of soot formation and the scientific evidence that supports this understanding. This talk will also cover the gaps in our understanding of soot chemistry, some reasons for these gaps, and what we may need to do in order to bridge these gaps and develop more insight into soot formation and evolution.

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Plenary IV: AEESP Lecture**This is Getting Dynamic: How the Volatility Basis Set Informs****Particle Formation and Growth.** NEIL DONAHUE, *Carnegie Mellon University*

A large fraction of atmospheric nanoparticle growth is driven by condensation of organic compounds. Especially below 10 nm there is a fine dance between curvature induced volatility enhancement (the Kelvin effect) and mixing (the Raoult effect). In addition to Koehler and nano-Koehler behavior, the distribution of organic volatility over a very wide range plays a key role in particle growth. A major contribution comes from the new (to atmospheric chemistry) process of peroxy-radical auto oxidation, which forms highly oxygenated organic molecules (HOMs) rapidly during the initial stages of oxidation. In the CERN CLOUD experiment we have been able to measure the full distribution of organic products in both the gas and particle phases, establishing closure between observed vapor concentrations, growth rates, and particle composition at temperatures ranging from 250 to 320 K. Finally, we observe interesting and potentially critical couplings between different organic peroxy radicals that may have major implications for the behavior of atmospheric organics in low-NO_x environments. All of these issues are well-suited to a dynamical version of the Volatility Basis Set that resolves peroxy-radical chemistry and provides a framework to describe the dynamics of organic particle nucleation and growth.

1AC.1

Autoxidation of Peroxy Radicals Formed from OH Radical-initiated Reactions of Trimethylbenzenes. Yuwei Wang, Archit Mehra, Jordan Krechmer, Andrew Lambe, Francesca Majluf, Douglas Worsnop, Manjula Canagaratna, Hugh Coe, LIN WANG, *Fudan University*

Secondary organic aerosols (SOAs) are formed in the atmosphere by oxidation of volatile gas-phase organic compounds, and have significant influence on human health and ecosystems. Highly oxygenated organic molecules (HOMs) are characterized with extremely-low volatility and thus are thought to be important precursors for SOA. However, traditional oxidation mechanisms initiated by OH radicals show a slow overall oxidation process, which don't support the observed rapid formation of HOMs. In this study, we performed lab experiments to investigate the autoxidation of peroxy radicals produced from trimethylbenzenes, which are common anthropogenic aromatic emissions in urban environments. An OH-radical initiated, highly oxidizing environment that simulates atmospheric oxidation processes on timescales of days was achieved with a potential aerosol mass (PAM) oxidation flow reactor. A FIGAERO-Iodide-L-ToF-CIMS and a Vocus® PTR-MS were applied to measure the particulate products and gas-phase products, respectively. Strong evidence in favor of the extensive existence of autoxidation of aromatics were obtained.

1AC.2

Chlorine-Initiated Photo-Oxidation of α -Pinene Under High NO_x Conditions: Oxidation Pathways, Product Distribution and Partitioning Behavior. CATHERINE MASOUD, Lea Hildebrandt Ruiz, *University of Texas at Austin*

Previous work has focused on quantifying the SOA-formation potential of α -pinene when oxidized by hydroxyl (OH) radicals or ozone (O₃), yet the effect of chlorine radicals (Cl) as oxidizing agents has not received much attention. Recent ambient measurements have shown that Cl can substantially affect SOA formation in continental as well as coastal regions. In this work, we focus on Cl-initiated photo-oxidation of α -pinene leading to the formation of oxidized products including SOA.

We report the SOA-formation potential of α -pinene + Cl under different experimental conditions including different NO_x levels, temperatures and VOC precursor concentrations. Compared to OH-oxidation, SOA formation is much faster for Cl-initiated oxidation and SOA yields are doubled. Moreover, the mass yields of α -pinene photo-oxidation by Cl are almost doubled under low NO_x conditions compared to high NO_x conditions.

We use a filter inlet mounted onto a High-Resolution Time-of-Flight Chemical Ionization Mass Spectrometer (FIGAERO-CIMS) to monitor the gas- and particle-phase products and identify several chlorinated species. Of these, we find several chlorinated- auto-oxidation products or highly oxygenated organic molecules (Cl-HOMs) including C₁₀H₁₃ClO₄, C₁₀H₁₅ClO₆, C₁₀H₁₅ClO₈. We propose mechanistic pathways for their occurrence, and we investigate their formation under different conditions. Our analysis shows that the formation of HOMs is enhanced under low NO_x (consistent with the higher SOA yields observed) and high temperature conditions. We also compare the abundance of HOMs in Cl- versus OH-initiated oxidations. Finally, we use the FIGAERO-CIMS to investigate gas-particle partitioning of oxidation products under different experimental conditions.

1AC.3

Atmospheric Chemistry of Volatile Chemical Products. REINA BUENCONSEJO, Sophia Charan, Christopher Kenseth, Paul Wennberg, John Seinfeld, *California Institute of Technology*

Recent work has indicated the growing importance of volatile chemical products (VCPs), particularly as air pollution regulations drive down the contribution of vehicular-based emissions. Thus, it is important to characterize the effects of VCP on atmospheric secondary organic aerosol (SOA) and its formation in order to better resolve discrepancies between SOA observations and models. This work looks at specific chemical mechanisms that lead to SOA formation and growth from VCP precursors. Compounds such as benzyl alcohol, n-butyl acetate, ethylene glycol butyl ether, and D5-siloxane were selected based on consultation with the California Air Resources Board (CARB). Analysis of these compounds is two-fold. First, molecular composition of the samples taken within the first 5 hours and after 5 hours of aerosol growth facilitated by aerosol seed are analyzed by an ultra-performance liquid chromatography/electrospray ionization quadrupole time-of-flight mass spectrometer (UPLC/ESI-Q-TOF-MS). This analysis determines the oxidation products that result in SOA formation. Secondly, oxidation of the VCP compounds in the absence of aerosol seed is studied via custom-built gas chromatography-chemical ionization mass spectrometer (GC-CIMS) to identify oxidation products. Both classes of experiments are carried out at different NO_x conditions so that an intercomparison of the different compounds can be made to better understand how NO_x and VCP structure affect the oxidation mechanisms.

1AC.4

The Effect of OH Scavengers on the Particle Phase Composition of α -Pinene Secondary Organic Aerosol. DAVID BELL, Veronika Pospisilova, Amelie Bertrand, Dongyu S. Wang, Chuan Ping Lee, Felipe Lopez-Hilfiker, Claudia Mohr, Wei Huang, Imad El Haddad, Jay G. Slowik, Andre S.H. Prévôt, Josef Dommen, Urs Baltensperger, *Paul Scherrer Institute*

OH scavengers (e.g. H_2 , CO, butanol, cyclohexane) have been used to consume all of the OH radicals that are formed in the reaction between an alkene and ozone. This is advantageous because the scavenger effectively shuts down a competing oxidation pathway so the resulting gas and particle phase products result from a single oxidation process. However, the impact a scavenger has on the resulting oxidation products has not been studied in depth until recently. Recent laboratory studies have showed that some dimers are suppressed when an OH scavenger is used in the ozonolysis of β -pinene.

In this study, experiments were performed in a series of atmospheric simulation chambers and a flow tube at the Paul Scherrer Institute studying the secondary organic aerosol formed from α -pinene + O_3 with various OH scavengers (butanol, cyclopentane, and cyclohexane). The particle phase products were monitored with an extractive electrospray ionization time-of-flight mass spectrometer (EESI-TOF), a soft ionization technique that measures real-time, near-molecular-level SOA composition.

The main constituents in the particle phase are $\text{C}_{10}\text{H}_x\text{O}_y$ species (where $x = 14, 16, \text{ and } 18$ and $y = 3 - 10$). $\text{C}_{10}\text{H}_{18}\text{O}_y$ products have been identified as products from OH chemistry via OH addition to the alkene, and subsequent auto-oxidation occurring. The $\text{C}_{10}\text{H}_{18}\text{O}_y$ fraction decreases by 50 - 70% when 200 ppm of butanol is present. The remaining $\text{C}_{10}\text{H}_{18}\text{O}_y$ left over is $y = 4$, corresponding to the Criegee intermediate reacting with H_2O . As a result, the monomer region demonstrates that butanol is effective at scavenging the OH produced in the reaction between α -pinene + O_3 . However, the dimer distribution of α -pinene SOA was completely altered when an OH scavenger was used. This was further studied with a series of flow tube experiments to gain insight about dimer formation in these systems.

1AC.5

Secondary Organic Aerosol Formation from Healthy and Aphid-Stressed Scots Pine Emissions. CELIA FAIOLA, Iida Pullinen, Angela Buchholz, Fatemeh Khalaj, Arttu Ylisirniö, Eetu Kari, Pasi Miettinen, Jarmo Holopainen, Minna Kivimäenpää, Siegfried Schobesberger, Taina Yli-Juuti, Annele Virtanen, *University of California, Irvine*

One barrier to predicting biogenic secondary organic aerosol (SOA) formation in a changing climate can be attributed to the complex nature of plant volatile emissions. Plant volatile emissions are dynamic over space and time, and change in response to environmental stressors. Emission rates and volatile composition are expected to evolve as the climate changes and causes plants to experience an increased level of stress. One important plant stressor in a warming boreal forest environment is insect herbivory as insect outbreaks increase in frequency and intensity. This study investigated SOA production from emissions of healthy and aphid-stressed Scots pine saplings via dark ozonolysis and photooxidation chemistry. Plant volatiles were transported to a batch reaction chamber where oxidation products and SOA production were monitored for a minimum of seven hours with the following instrumentation: PTR-ToF-MS, acetate-CIMS, aerosol mass spectrometer, and scanning mobility particle sizer. The initial volatile mixture in the chamber was characterized via cartridge sampling and off-line analysis on a thermo-desorption gas chromatograph mass spectrometer (TD-GC-MS). The initial volatile mixture from healthy plants included monoterpenes, aromatics, and a small amount of sesquiterpenes. The biggest change in the volatile mixture for aphid-stressed plants was a large increase in sesquiterpene emissions—particularly acyclic sesquiterpenes, such as the farnesene isomers. Oxidation products measured with an acetate-CIMS will be presented with estimated volatility distributions. Potential mechanisms accounting for changes in SOA mass yield between different chemical mechanisms and healthy vs. stressed plant volatile mixtures will be discussed.

1AC.6

Estimating Vapor Wall-Loss to Improve Organic Aerosol Volatility Distributions. KERRIGAN CAIN, Eleni Karnezi, Spyros Pandis, *Carnegie Mellon University*

Vapor wall-loss has been shown to be an important process in smog chamber studies, especially in yield experiments where organic aerosol (OA) concentrations can be underestimated due to semi-volatile vapor losses to chamber walls. Vapor wall-losses are also important, but largely unaccounted for, in active dilution experiments because an evaporating particle-phase component may never be able to fully reach equilibrium if the corresponding vapor-phase component is continually lost to the chamber walls. This study presents results that account for vapor wall-losses in a dilution chamber and estimate volatility distributions of secondary OA (SOA) generated from the ozonolysis of α -pinene and cyclohexene during experiments combining thermodenuder (TD) and isothermal dilution measurements.

In this study, SOA was generated in a main chamber and characterized with a TD. The SOA was also isothermally diluted in a smaller dilution chamber. After correction for particle wall-losses, we generated thermograms and areograms, particle mass fraction remaining as a function of TD temperature or time in the dilution chamber. We then used a dynamic mass transfer model coupled with an error minimization approach to estimate the SOA volatility distributions. However, the model was updated in this work to account for and estimate vapor wall-losses occurring in the dilution chamber. The model results indicated that the bulk vapor wall-loss constant for this chamber and the SOA species studied was ~ 0.3 h^{-1} and, when compared to model results that did not account for vapor wall-losses, significantly reduced the uncertainty in the volatility distributions and corresponding properties. In addition, the model predicted that some semi-volatile compounds can completely evaporate from the particle-phase due to vapor wall-losses. This work signifies the importance of accounting for vapor wall-losses to accurately estimate OA volatility.

1AC.7

Detailed Comparison of Chamber Measurements and Mechanistic Predictions to Improve Understanding of SOA Formation Mechanisms. JOSHUA MOSS, Abigail Koss, Kevin Nihill, Martin Breitenlechner, Alexander Zaytsev, Richard Valorso, Marie Camredon, Bernard Aumont, Frank Keutsch, Jesse Kroll, *MIT*

Elucidating the underlying chemical mechanisms pertaining to Secondary Organic Aerosol (SOA) formation and evolution via the oxidation of Volatile Organic Compounds (VOCs) is critical to improving our understanding of organic matter in the atmosphere. Much of our understanding of such mechanisms derives from experimental studies such as chamber experiments coupled with mass spectrometric measurements of the chemical composition of the gas and particle phases. These provide time-resolved measurements of individual species as well as measurements of ensemble properties such as elemental ratios and SOA yields. However, such measurements have inherent limitations such as those arising from the influence of walls and surfaces, and there are significant challenges associated with the interpretation of mass spectra in terms of detailed molecular composition. On the other hand, detailed chemical mechanisms enable the prediction of concentration profiles for a wide range of chemical species, but they are limited by a priori knowledge of the underlying chemistry and have not always been validated against experimental data. In this study, we carry out a detailed comparison of measured oxidation products (from a series of chamber studies) and results from a self-generating chemical mechanism (GECKO-A) in order to improve our understanding of the oxidation mechanisms of multiple VOCs. The chamber experiments were conducted with a suite of instruments that measured the majority of the product organic carbon in both the particle and gas phases. This enables the direct comparison with GECKO-A predictions, across various levels of detail, ranging from ensemble properties such as oxidation state and SOA yields to more granular data such as time series of individual molecular species. This comparison helps inform both the measurements and the model: differences between the predicted and measured results can suggest edits to the model (e.g., improved branching ratios) while model results can help clarify and disambiguate chamber mass spectrometry data and help constrain physical processes such as partitioning among the gas, particles, and walls. The ultimate objectives of this work are to yield novel insights into SOA oxidation mechanisms while also providing a template for future model-measurement comparisons.

1AD.1

Analysis of Nanoparticle Toxicity at the Air-Liquid Interface of Lung Cells. TREVOR TILLY, Ryan Ward, Alyssa Morea, Sarah Robinson, Arantazu Eiguren Fernandez, Tara Sabo-Attwood, John Lednicky, Chang Yu Wu, *University of Florida*

A bioinspired lung cell exposure system for toxicity analyses of nanoparticles, Dosimetric Aerosol in Vitro Inhalation Device (DAVID), was shown to have enhanced particle deposition efficiency through a physiologically relevant mechanism known as condensational particle growth. Condensational particle growth increases the size of aerosolized nanoparticles through the condensation of water vapor onto their surface, which amplifies particles as small as 10 nm in diameter to uniform micron-sized droplets, and this results in a gain inertia of particles in motion. Epithelial lung cells were cultured and exposed at the air-liquid interface (ALI) to CeO₂ and CuO aerosols generated by a Collision nebulizer and an acoustic powder disperser. Use thereof resulted in distinct particle size distributions and a ten-fold difference in exposed aerosol mass concentration. CeO₂ and CuO aerosols generated by the nebulizer resulted in high number concentrations (>10⁶ #/cm³) with mean diameters similar to their primary particle sizes of 33.3±1.18 nm and 50.9±7.10 nm, respectively. The CeO₂ and CuO aerosols generated by the acoustic disperser had a lower number concentration, but greater mass concentration than the nebulizer exposures, which resulted from their larger aerodynamic diameters of 3.06±0.45 μm and 2.25±0.07 μm, respectively. ALI cellular exposure to the CeO₂ aerosol did not result in significant toxicity at a nebulizer dose level of 12.5 μg/cm² or at the acoustic dose level of 109 μg/cm². In contrast, exposing cells cultured at the ALI to CuO aerosols resulted in a dose dependent cellular membrane toxicity at all exposure concentrations (4.1 to 65 μg/cm²). Furthermore, submerged cells exposed to CeO₂ nanoparticles did not reduce cell viability, but exposure to 20 μg/mL of CuO resulted in greater than 50% decrease in mitochondrial activity. The findings indicate a potential difference in the toxicity mechanisms for cells exposed to particles as an aerosol and under submerged culture conditions.

1AD.2

Synergistic and Antagonistic Interactions Among the Particulate Matter (PM) Components for Cellular ROS activity and Cytotoxicity. YIXIANG WANG, Joseph V Puthussery, Haoran Yu, Vishal Verma, *University of Illinois Urbana-Champaign*

Several studies have shown the associations of ambient particulate matter (PM) concentrations with many adverse health effects. The oxidative potential (OP) of PM is hypothesized to be one of the important parameters associated with its toxicological effects. To study the OP, researchers have used chemical approaches to mimic the reactive oxygen species (ROS) generation catalyzed by PM in the cells or the lung fluid. Many chemical assays have been applied to investigate the interactions among various PM components for the generation of ROS. However, their results haven't been verified by the cellular assays. In this study, we have chosen three metals (Cu, Fe, and Mn) and four quinones (9,10-phenanthraquinone, 1,2-naphthoquinone, 1,4-naphthoquinone, and 5-hydroxy-1,4-naphthoquinone), that are most abundant in PM, in addition to the ambient humic-like substances (HULIS) from the real PM samples. We exposed the Chinese hamster ovary (CHO) cells to the mixtures of these components for 72 hours to assess the cytotoxicity and obtained the lethal concentration that causes 50% inhibition (LC50). Mixture toxicity index (MTI) method was used to determine the interaction. The MTI result indicates that Fe is synergistic with most quinones and HULIS in cytotoxicity. The interactions among quinones are mostly additive. To assess the contribution of OP in cytotoxicity, we further studied these interactions by an intracellular ROS assay, which demonstrate a similar pattern. Most importantly, we found a strong correlation between the intracellular ROS and LC50 ($R^2 = 0.67$; $N = 20$), which indicates that the interaction among the PM components for cellular ROS activity is probably responsible for the observed cytotoxicity.

1AD.3

CYCLEX: Cyclone Collection of Particulate Matter Followed by Exposure Experiments. TOMOAKI OKUDA, Takaaki Goto, Hirohisa Takano, Akiko Honda, Toshinori Onishi, Michitaka Tanaka, Shuichi Hasegawa, Takayuki Kameda, Susumu Tohno, Chiharu Nishita-Hara, Keiichiro Hara, Masahiko Hayashi, Koza Inoue, *Keio University*

Numerous epidemiological studies have reported adverse health effects due to aerosols. In particular, allergic rhinitis and bronchial asthma in addition to cardiovascular diseases are seriously concerned. However, detailed mechanisms of the cellular biochemical reactions associated with the toxicity of aerosol particles have not been elucidated well so far. Cell exposure studies for aerosol particles have often been conducted using particulate matter collected by vibrating/scraping aerosol-loaded filters. However, the amount of particles that are collected on a filter is often insufficient to perform an exposure studies. In this study, a high-volume simultaneous sampler for fine and coarse aerosol particles was developed using the impactor and cyclone techniques. The newly developed instrument allows researchers to collect a sufficient amount of aerosol particles for exposure studies without using filters. We collected fine and coarse aerosol particles in three cities (Yokohama, Saitama, and Fukuoka) in Japan under the CYCLEX (Cyclone collection of PM followed by Exposure Experiments) project. Chemical analysis of the collected particles has been carried out for carbonaceous materials (EC and OC), water-soluble ionic species, metals, and PAHs, then followed by cellular exposure experiment. We found particle size- and sampling location-dependent response in the results of exposure experiments. Both fine and coarse particles collected at all locations decreased the viability of nasal epithelial cells and antigen presenting cells (APCs), increased the production of IL-6, IL-8, and IL-1 β from bronchial epithelial cells and APCs, and induced expression of dendritic and epithelial cell (DEC) 205 on APCs. Several chemical components showed significant correlations to inflammatory responses or cytotoxicity. These results suggest that ambient fine and coarse particles differently affect upper and lower respiratory tract and immune response, which may depend on their diameter, the components, and other parameters caused by the difference in collection location.

1AD.4

How Realistic Are In-Vitro Doses Used for Particle Toxicity Studies: Is There Something “Wrong” with Our In-Vitro Assays? OTMAR SCHMID, *Helmholtz Zentrum München*

There is an apparent gap between onset doses of inhaled particle toxicity observed in in-vitro cell and in-vivo animal models of the lung. Typically, in-vitro assays are much less sensitive than animal models when considering tissue-delivered dose. I will show that many cell cultures assays do not even respond after receiving equivalent lifetime doses for realistic exposure scenarios.

In this talk a strategy for direct comparison of in-vitro and in-vivo dose-response curves will be presented, typical onset doses as reported by in-vitro and in-vivo studies with soot and engineered nanoparticles will be compared and several hypothesis for the apparently low sensitivity of cell culture models will be discussed. This will provide insight into future perspectives of in-vitro particle toxicity studies and their relevance for assessing health risks due to exposure to inhaled particles.

1AD.5 (INVITED)

Assessing Exposures and Health Effects of Ambient Particle Radioactivity: An Emerging Field for Investigation by Aerosol Researchers. PETROS KOUTRAKIS, *Harvard T.H. Chan School of Public Health*

Exposure to radon (Rn) gas and its decay products (progeny) is common, with an estimated 7.1 million U.S. homes above the Environmental Protection Agency (EPA) Rn mitigation level of 4 pCi/L, which is an action level based only on lung cancer risk. To date very little is known whether exposure to Rn and its progeny causes other adverse effects. We hypothesize that α -radiation emitted by Rn progeny attached to ambient or indoor particles PM_{2.5} or PM₁₀ causes adverse cardiovascular and respiratory effects.

Our novel scientific premise regarding the enhancement of air pollution particle toxicity by Rn progeny is firmly supported by recent studies. During my presentation I will give an overview of these investigations. This will include findings from two national studies identifying radon as a potential cardiovascular and respiratory mortality risk. Next, I will introduce new exposure metrics of particle radioactivity and their association with blood pressure, lung function, and inflammatory markers in two cohort studies. Finally, I will present methods to assess indoor levels of particle radioactivity and to measure radon progeny in human tissues.

1AD.6**A Historical Perspective on Evaluation of Health Hazards of Airborne Plutonium.** ROGER MCCLELLAN, *Private Consultant*

Seaborg in 1940 used the University of California-Berkeley (UC-B) cyclotron to discover a new element – Plutonium (Pu). It was soon recognized that ^{239}Pu could be used to build a nuclear fission bomb. This led to the Manhattan Project and production of ^{239}Pu in uranium-fueled reactors. Seaborg was aware exposure to alpha particle emissions from naturally occurring radionuclides caused lung cancer in Uranium miners and bone cancer in Radium dial painters. Thus, he recognized exposure to ^{239}Pu could pose a serious health hazard leading him to provide aliquots of the first weighable quantities of ^{239}Pu to UC-B colleagues to investigate fate and toxicity of ^{239}Pu in laboratory animals. Results of these studies in combination with data from the radium dial painters were used in 1944 to set radiation protection standards for Pu workers. After World War II, research programs on the toxicity of Pu were initiated at the University of Utah, the Hanford Laboratories and the Lovelace Inhalation Toxicology Research Institute. These programs initially focused on ^{239}Pu and later expanded to include ^{238}Pu used as a thermal source in Space Nuclear Auxiliary Power systems. In 1967, a Registry of Pu workers in the USA was initiated. The multi-faceted research conducted over the past 75 years has made substantial contributions to understanding health hazards of Pu. Moreover, this research has contributed to understanding the mechanisms of toxicity of all kinds of airborne materials. The Radiation Protection Standards and work practices introduced in 1944 proved effective in protecting USA workers. Unfortunately, in Russian poor hygienic conditions led to an increased incidence of cancers in lung, liver and skeleton of Pu works validating the results observed in laboratory animals. This remarkable experience with Pu provides valuable lessons for addressing the potential human health hazards of other man-made agents.

1BC.1**Particulate Matter and Black Carbon from an LPG Stove Intervention in Rural Households in Puno, Peru: Preliminary Results.** MAGDALENA FANDIÑO-DEL-RIO, Josiah Kephart, William Checkley, Kirsten Koehler, *Johns Hopkins Bloomberg School of Public Health*

Household air pollution (HAP) from biomass fuels is a leading risk factor for preventable diseases and among the largest environmental contributors to the global disease burden. Previous interventions with improved cookstoves have not markedly lowered concentrations and therefore show only limited improvements on health. As a result, recent efforts are focusing on stoves that use cleaner fuels such as liquefied petroleum gas (LPG).

A randomized controlled field trial enrolled 180 female participants and followed them for one year. Free LPG stoves and fuel were delivered to 90 participants. We collected 48-hour measurements of kitchen concentrations and personal exposure to fine particulate matter ($\text{PM}_{2.5}$) and black carbon (BC). Household kitchen characteristics and their influence on concentrations were also evaluated. Baseline mean daily average kitchen concentrations and personal exposures of $\text{PM}_{2.5}$ of $1,200 \mu\text{g}/\text{m}^3$ ($\text{SD}=945 \mu\text{g}/\text{m}^3$) and $120 \mu\text{g}/\text{m}^3$ ($\text{SD}=175 \mu\text{g}/\text{m}^3$) respectively, were observed among biomass fuel users ($n=178$). After the LPG stove intervention, we observed average reductions of approximately 90% in kitchen concentrations and 75% for personal exposures to $\text{PM}_{2.5}$ on quarterly visits compared to baseline concentrations ($n=170$). BC concentrations were reduced in kitchens by 85% and personal exposures reduced by 65% ($n=170$). Preliminary results show not only sharp concentration reductions expected from good initial compliance, but also sustained reductions from the LPG stove use even after 12 months of the LPG stove intervention.

Results from this analysis will provide valuable information to help understand PM and BC exposure from biomass fuel use and changes that follow the adoption of LPG stoves. Results of this trial will inform the feasibility of an LPG stove replacement program to reduce HAP and improve health in resource-limited settings such as Peru.

1BC.2

Pellet-fed Gasifier Stoves Approach Gas-stove Like Performance during In-home Use in Rwanda. WYATT CHAMPION, Ky Tanner, Andrew Grieshop, *North Carolina State University*

Nearly all households in Rwanda burn solid fuels for cooking. A private firm in Rwanda is distributing forced-draft pellet-fed semi-gasifier cookstoves and fuel pellets. We measured in-use emissions of pollutants including fine particulate matter ($PM_{2.5}$), organic and elemental carbon (OC, EC), black carbon (BC) and carbon monoxide (CO) in 91 uncontrolled cooking tests (UCTs) of both pellet and baseline (wood; charcoal) stoves. We observed >90% reductions in most pollutant emission factors/rates from pellet stoves compared to baseline stoves. Pellet stoves performed far better than gasifier stoves burning unprocessed wood, and consistent with ISO tiers 4 and 5 for $PM_{2.5}$ and CO, respectively. Pellet stoves were generally clean, but performance varied; emissions from the dirtiest pellet tests matched those from the cleanest traditional stove tests. Our real-time data suggest that events occurring during ignition and the end of testing (e.g., refueling, char burnout) drive high emissions during pellet tests; these “non-ideal” modes were recreated during controlled laboratory ‘stress-testing’ that partially explain field results and may be useful for stove designers. Additionally, we use our field data to estimate potential health and climate cobenefits from stove adoption. This analysis suggests that pellet stoves, when operated correctly, have the potential to provide health benefits far above previously tested biomass stoves and approaching modern fuel stoves (e.g., LPG). Net climate impacts of pellet stoves range from similar to LPG to negligible, depending on biomass source and upstream emissions.

1BC.3

Coupling Laboratory and Field Measurements to Estimate Air Pollutant Emissions from Cookstoves. KELSEY BILSBACK, Rose Eilenberg, Lauren Hoskovec, Michael Johnson, Jack Kodros, Eric Lipsky, Christian L'Orange, Jessica Tryner, Ander Wilson, Allen Robinson, Jeffrey R. Pierce, John Volckens, *Colorado State University*

Air pollution from solid-fuel combustion in cookstoves is a leading cause of death and disease worldwide. Currently, emissions measurements used for indoor and outdoor air quality modeling are primarily derived from laboratory experiments; however, most laboratory-derived data underestimate the magnitude and variability of emissions measured during in-home cooking practices. Contrastingly, data collected during in-home cookstove use are realistic; however, field campaigns are logistically difficult, cost prohibitive, and only provide a limited view of emissions within a specific home or region. To address these gaps, we developed methodology that combines (1) statistical models trained on laboratory data and (2) low-cost in-field measurements to estimate fine particulate matter ($PM_{2.5}$), carbon monoxide, and black carbon. Multiple statistical model forms, with varying complexity, were tested to identify which models could provide the most accurate emissions estimates based on the lowest in-field measurement costs. The models utilized several forms of firepower and modified combustion efficiency (MCE) as predictors. To validate the models, we collected emissions measurements and continuous firepower and MCE measurements from cookstoves in Honduras, Uganda, and India. Continuous firepower was estimated using temperature at the combustion chamber outlet and MCE was estimated using a low-cost gas analyzer. When comparing our model-based estimates to emissions measurements taken in the field, we find that the model estimates are generally accurate enough to predict the International Standards Organization (ISO) emissions tier a given stove will operate at in the field. We also find that including both firepower and MCE measurements in the model, rather than firepower alone, can improve the accuracy of the model-based emissions estimates by 63%. Although further validation is needed, our methodology, which combines laboratory-derived statistical models and minimal in-field monitoring, shows promise for estimating emissions levels observed in the field.

1BC.4

Development of Volatility Distributions of Biomass Burning Organic Emissions. ADITYA SINHA, Ingrid George, Amara Holder, Michael Hays, Andrew Grieshop, *North Carolina State University*

The volatility distribution of organic emissions from biomass burning and other combustion sources is a key property in determining their atmospheric evolution due to partitioning and aging. The gap between measurements and models predicting secondary organic aerosol (SOA) has been attributed to the absence of semi- and intermediate volatility organic compound (S/IVOC) measurements. The contribution of S/IVOCs from biomass burning emissions, a significant source of atmospheric OA burden, often quantified via the volatility basis set (VBS) framework, is not well understood. There is uncertainty in the amount and composition of S/IVOCs and how they are influenced by factors like fuel type and combustion conditions. To address this, we collected sorbent tubes and quartz fiber filter samples from biomass burning experiments using a range of fuels and combustion approaches and analyzed them using thermal desorption gas chromatography-mass spectrometry (TD-GC-MS) for targeted and non-targeted analysis of compounds with a wide range of volatilities. Current research involves using the VOC and S/IVOC measurements from these experiments and projecting them onto the VBS framework to understand gas-particle partitioning from these sources. We will develop volatility distributions of the organic emissions from woodstoves used for domestic heating, samples from in-situ and simulated open burning and biomass cookstoves used in developing country households. We will conduct comparisons of VBS distributions within and across these sources to explore variability and identify any commonalities. We will also explore variation across the various fuel types, modified combustion efficiencies and appliance types and compare with speciated measurements and previous VBS distributions from the literature. The resulting volatility distributions and associated emission factors can be used to update emission inventories and simulate the gas-particle partitioning of biomass burning in chemical transport models.

1BC.5

Chemical Characterization of Biomass Burning Sources Using Targeted and Untargeted Approaches. CAMILLE NOBLET, François Lestremau, Marie Lemire, Jean-Luc Besombes, Jean-Luc Jaffrezo, Olivier Favez, Serge Collet, Alexandre Albinet, *INERIS, France*

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 the PM concentration levels is difficult and rarely achieved. Such discrimination is of major concern for air quality policy-makers in order to implement efficient 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 in a large combustion chamber facility (1000 m³) to simulate the ambient air dilution conditions. Different wood combustion appliances, such as a residential wood stove and a fireplace, under different output conditions (nominal vs reduced) and wood log moisture content (mix of species including beech, oak and hornbeam), have been tested. The green waste burning experiments have been carried out using two kinds of burning material such as grass mowing with tree leaves and hedge trimming with branches. Smoke temperature, O₂, NO_x, CO, CO₂, 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 (dilution factor about 500-1000). Filter samples have been characterized using both, targeted (EC/OC, levoglucosan and its isomers, PAHs, methoxyphenols, alkanes, polyols) and non-targeted (high resolution mass spectrometry analyses) approaches. Preliminary targeted results showed the predominance of higher molecular weight alkanes with odd carbon numbers (C₂₇, C₂₉, C₃₁) in the case of green waste burning versus open or closed fires. Results obtained showed that levoglucosan/mannosan ratios for green waste burning (<7) were significantly different than for residential heating (>17). For the non-target screening approach, which is not commonly used in the atmospheric chemistry, a description of the analytical development will be presented. Thanks to the chemical fingerprints obtained from GC/Q-TOF-MS and LC/Q-TOF-MS analyses and statistical data analysis, chemical pattern of each biomass burning source will be highlighted and will complete the information already provided by the targeted results to better discriminate both sources.

1BC.6

Constituents of Health Concern from Biomethane Cooking Stove Combustion Exhaust. CHAO WAN, Yin Li, Chris Alaimo, Jian Xue, Minji Kim, Norman Kado, Peter Green, Thomas Young, Ruihong Zhang, Michael Kleeman, *University of California, Davis*

Biogas is a promising source of renewable energy with composition similar to natural gas. Advances in anaerobic digestion methods and biogas purification technology will soon produce upgraded biogas (=biomethane) that can be used in any application where natural gas is used, including in residential cooking stoves where the potential for exposure to direct combustion exhaust is very high. Here we report the composition of biogas and biomethane including ammonia, extended hydrocarbon, sulfur, mercury, metals, bacteria, volatile and semi-volatile organic compounds from seven different biogas production streams. Among all the constituents, halocarbons and siloxanes were identified as contaminants of concern due to their potentially high concentrations and toxic combustion products. A series of controlled combustion experiments were conducted with a residential cooking stove using biomethane spiked with dichloromethane and 1,2-dichloro-1,1-difluoroethane to calculate the conversion rates of chlorine and fluorine becoming hydrochloric acid and hydrofluoric acid. D4 and D5 siloxanes were spiked into the fuel to study the formation and size distribution of silica nanoparticles. Our experiments show that all siloxanes are combusted to silica particles but the size distributions vary significantly depending on siloxane concentrations. A coagulation model is developed to describe this process. Pipeline standards are proposed for halocarbons and siloxanes based the experimental results.

1BC.7

Carbonaceous Semivolatile Organic Matter Emitted from a Pellet-fired Biomass Boiler. MICHAEL HAYS, John Kinsey, Ingrid George, William Preston, Carl Singer, Bakul Patel, *U.S. EPA*

Biomass pellets are an intriguing source of renewable energy; although, the air pollution and exposure risks posed by the emissions from burning pellets in biomass boilers are uncertain. The present study examines the carbon composition of fine particle matter (PM) emissions from a biomass boiler (OBB) firing switch grass and hardwood biomass pellets at different test cycles. The organic and elemental carbon (OC and EC) content and select semivolatile organic compounds (SVOCs) in filter-collected PM were identified and quantified using thermal-optical analysis and gas chromatography-mass spectrometry (GC-MS), respectively. Fine PM emissions from the OBB ranged from 0.4 g/kg to 2.91 g/kg of pellets burned of which $40\% \pm 17\%$ w/w was carbon. The sum of GC-MS quantified SVOCs in the PM emissions varied from 0.13 g/g OC to 0.41 g/g OC. Relatively high levels of oxygenated compounds were observed in the PM emissions, and the most predominant individual SVOC constituent was levoglucosan (12.5 mg/g OC - 320 mg/g OC). The effect of boiler test cycle on emissions was generally greater than the effect due to pellet fuel type. Organic matter emissions increased at lower loads owing to less than optimal combustion performance. Compared with other types of residential wood combustion, pellet burning in the OBB lowered PM emissions by nearly an order of magnitude. The PM emitted from burning pellets in boilers also contains comparatively less carbon; however, the toxic polycyclic aromatic hydrocarbons (PAH) in the PM from pellet-burning varied substantially, and produced 2-10 times more benzo[k]fluoranthene, dibenz[a,h]anthracene, and indeno[1,2,3-c,d]pyrene. These results suggest that further toxicological evaluation of biomass pellet burning emissions is required to properly understand the risks posed.

1CC.1**Deriving CCN from High-Spectral Resolution Lidar Measurements of Aerosol Extinction and Backscatter.**

RICHARD MOORE, Kyle Dawson, Sharon P. Burton, Snorre Stamnes, Richard Ferrare, Chris Hostetler, Luke Ziemba, Ewan Crosbie, Edward Winstead, Yohei Shinozuka, Kenneth Thornhill, Bruce Anderson, *NASA Langley Research Center*

Airborne field campaigns provide the means to develop and test correlations between CCN number concentrations and remote sensing observations of aerosol optical properties. There have been a number of such assessments in recent years (e.g., Andreae, 2009; Liu et al., 2014; Shinozuka et al., 2015), each with varying degrees of success. Here, we evaluate relationships between aerosol extinction and backscatter coefficients and in situ CCN spectra for a case study in the remote North Atlantic. It is found that in situ measurements reasonably capture aerosol loading on a number basis, but substantially under-sample the coarse mode aerosol that dominate the aerosol optical properties. Methods for unraveling this complexity to remotely sense the submicron aerosol fraction relevant for CCN will be discussed.

1CC.2**Cold Fronts Promote New Particle Formation over Mid-latitude Remote Oceans.**

GUANGJIE ZHENG, Yang Wang, Michel Jensen, Chongai Kuang, Isabel McCoy, Rob Wood, Alyssa Matthews, Fan Mei, Jason Tomlinson, Ewan Crosbie, Luke Ziemba, Richard Moore, Jian Wang, *Washington University in St. Louis*

The indirect effects of aerosols on clouds remain highly uncertain in predicting the future climate. Among the major contributions to this uncertainty is poor understanding of the formation, evolution, and transport of aerosols in the remote marine environment, where the albedo and lifetime of low clouds are highly susceptible to perturbations in aerosol properties. Globally, new particle formation (NPF) represents an important source of aerosol and cloud condensation nuclei (CCN). Model simulations show that nearly half of the global CCN in the planetary boundary layer may be formed through NPF.

In this study, aerosol properties and processes over the Eastern North Atlantic (ENA) are examined using measurements onboard the US Department of Energy Gulfstream-1 (G-1) research aircraft during the Aerosol and Cloud Experiments in the Eastern North Atlantic (ACE-ENA) campaign and long-term observation at the Atmospheric Radiation Measurement (ARM) ENA site on Graciosa Island. NPF was observed in lower free troposphere (FT) and upper decoupled layer within the marine boundary layer (MBL) following the passage of cold front, which is often associated with convective clouds and intense precipitation. The convective clouds transport ocean-emitted gas precursors upward to the upper decoupled layer and lower FT, and aerosol surface area concentrations are reduced due to wet deposition, leading to NPF. In addition, reduced temperature and relatively lower cloud fraction (i.e., stronger radiation and therefore photochemical activities) following the cold front passage also facilitate NPF. Following the passage of a cold front, the newly formed particles in the upper decoupled layer are transported downwards into the surface mixed layer, where they grow and may become CCN. The influence of post cold front NPF on the population of MBL aerosols and CCN budget will be discussed.

1CC.3

Geoengineering for Climate Change: Nature Has Already Demonstrated the Process and Effects. RUSSELL SCHNELL, *National Oceanic and Atmospheric Administration*

Geoengineering to reduce atmospheric air temperatures is becoming a hot topic with recent articles in *Science*, *Nature* and the *Bulletin of the American Meteorological Society* discussing the pros, cons and methods of “solar engineering.” A proposed method is to inject millions of tons of sulfur dioxide or calcium carbonate into the stratosphere to reflect solar radiation back to space.

Through volcanic eruptions that spewed mineral particles and sulfur dioxide into the stratosphere, nature has provided excellent examples of geoengineering: El Chichon, Mexico (29 March, 1982, ~7 MT) and Mount Pinatubo, Philippines (June 14, 1991, ~20 MT).

Reductions in solar radiation measured at the Mauna Loa Atmospheric Baseline Observatory (MLO), Hawaii from these eruptions showed a 14% reduction from El Chichon and 11% reduction from Pinatubo at the peak of the stratospheric aerosol loadings. Lidar measurements of the eruption aerosols showed they were concentrated between 15 and 30 km altitude and took 4-5 years to return to background levels. These aerosols reduced northern hemisphere temperatures by ~0.5°C for Pinatubo and ~0.7°C for El Chichon.

NOAA WP-3 aircraft measurements in the Arctic stratosphere off Greenland, one year after the El Chichon eruption, collected crustal debris in the 10⁰ to 10¹ micron diameter range in concentrations of 10⁻³ to 10⁻² cm⁻³ and H₂SO₄ droplets in the 10⁰ to 10⁻¹ micron diameter range in concentrations of 10⁻¹ to 10² cm⁻³.

Peak aerosol optical depth anomalies measured at MLO were 0.2 for both El Chichon and Pinatubo aerosols and 0.17 and 0.21 respectively at the Barrow, AK, Baseline Observatory (BRW). From NOAA WP-3 measurements in the stratosphere over BRW on April 22, 1992 (Pinatubo, 10 months post-eruption), stratospheric aerosol depth was in the 0.19 to 0.2 range.

1CC.4

Size-Dependent Nanoparticle Growth Profile from CLOUD Experiments. WEIMENG KONG, Stavros Amanatidis, Dongyu S. Wang, Loïc Gonzalez Carracedo, Birte Rörup, Dominik Stolzenburg, Jasper Kirkby, John Seinfeld, Richard Flagan, *California Institute of Technology*

New particle formation (NPF) from gaseous precursor vapors is frequently observed in the ambient environment and contributes to a major source of global cloud condensation nuclei (CCN). The survival and activation rate of newly formed particles are highly dependent on particle growth below 10 nm. Therefore, characterizing and understanding nanoparticle early growth can help to quantify the impact of NPF on the global CCN budget.

We performed a number of experiments under various atmospheric conditions in the Cosmics Leaving Outdoor Droplets (CLOUD) chamber at the European Organization for Nuclear Research (CERN) to better understand NPF, particle growth and survival. Multiple experimental parameters were varied to study the influence of different highly oxygenated molecules (HOMs) and inorganic trace gases, such as ammonia and nitrogen oxides on particle early growth.

This work reports particle sizing and growth results measured by the Caltech nano-scanning electrical mobility analyzer (nSEMS), which measured continuous particle size distributions from 1.5 nm to 25 nm. The transfer function of nSEMS was derived based on electric and flow field simulations and validated with empirical measurements. Nanoparticle early growth was also modelled as gas-to-particle condensational growth to compare with experimental measurement. In order to capture the full picture of nanoparticle growth, survival and activation, size distribution information from the nSEMS were also compared and combined with other particle sizing instruments from CLOUD to obtain a continuous particle growth profile over the range from 1 nm to 500 nm.

1CC.5

Wintertime New Particle Formation and Its Contribution to Cloud Condensation Nuclei in the Northeastern United States. FANGQUN YU, Gan Luo, Yanda Zhang, James Schwab, Joseph P. Marto, Lauriana C. Gaudet, Kara Sulia, *The State University of New York at Albany*

Particle number concentration is an important factor affecting the health and climate impacts of atmospheric aerosols. For example, high number concentrations of ultrafine particles may lead to adverse health effects. Atmospheric particles act as cloud condensation nuclei (CCN) and modify cloud properties and precipitation and thus indirectly impact the hydrological cycle and climate. New particle formation (NPF), frequently observed at various locations around the globe, is an important source of ultrafine particles and CCN in the atmosphere. In this study, wintertime particle formation over the northeastern United States (NEUS) is simulated with WRF-Chem coupled with a size-resolved (sectional) advanced particle microphysics (APM) model. Model simulated variations of meteorology, aerosol precursors, and particle number concentrations agree well with corresponding measurements taken at Pinnacle State Park, NY. We show that even during wintertime, regional nucleation occurs and contributes significantly to ultrafine particle and CCN number concentration in NEUS. Due to low biogenic emissions, wintertime regional nucleation is solely controlled by inorganic species and the newly developed ternary ion-mediated nucleation is able to capture the variations of observed particle number concentrations (ranging from $\sim 200 - 20,000 \text{ cm}^{-3}$). Sulfuric acid, ionization and ammonia are major parameters controlling NPF in the NEUS wintertime, which contributes to more than 90% of total particle number concentrations and $\sim 50\%$ of CCN and cloud droplet number concentrations. The impact of NPF on cloud and ice water content and precipitation will also be discussed.

1CC.6

Understanding and Modeling Sources of Ice Nucleating Particles in Earth System Models. SUSANNAH BURROWS, Christina McCluskey, Xiaohong Liu, Paul DeMott, *Pacific Northwest National Laboratory*

Sea-spray aerosol is enriched in marine organic matter originating from phytoplankton. Although the complex biology and chemistry controlling the emitted aerosol is not yet fully understood, sea spray organic matter may alter the magnitude of sea spray emissions, and enable sea spray to act as a source of ice nucleating particles (INPs). OCEANFILMS (Burrows et al., 2014) is an approach to modelling the relationship between ocean biogeochemistry and emitted sea spray aerosol chemistry for Earth System Models, which has recently been implemented in version 1 of the Energy Exascale Earth System Model (E3SMv1), developed by the U.S. Department of Energy (Burrows et al., ACPD, in revision). The conceptual approach of OCEANFILMS will be described and impacts on simulated aerosols and clouds will be highlighted.

In a related study, we have evaluated the potential of a current global Earth System Model to skillfully simulate observed boundary-layer INP concentrations at coastal and marine locations (McCluskey et al., submitted). The OCEANFILMS parameterization was implemented into version 1 of the Community Earth System Model (CESM1), and a recently-developed active site density parameterization for marine INP (McCluskey et al., 2018) was applied to calculate the INP concentrations from simulated sea spray aerosol. Simulated dust INP were parameterized as well (DeMott et al., 2015). Nudging of atmospheric winds was used to match observed meteorology during two recent field campaigns – a coastal campaign at Mace Head, Ireland, and a shipboard campaign in the Southern Ocean. The resulting INP concentrations were compared with observed INP concentrations. Agreement with observations was improved by including sea spray INPs, and sea spray aerosol was a dominant contributor to the INP population at cloud-relevant altitudes. This study demonstrates the need to account for INPs associated with sea spray aerosol and their subsequent influence on cloud phase transitions.

1CC.7

Morphology and Optical Properties of Soot. Georgios Kelesidis, SOTIRIS E. PRATSINIS, *ETH Zurich*

There is renewed interest in understanding the detailed structure and optical properties of soot as it is the second largest contributor (after CO₂) to radiative forcing. In addition, soot exhibits by far the largest uncertainty (90%) of all such contributors. Furthermore, this understanding is still sought for reliable monitoring of soot emissions, carbon black processing and fire detection. Here, soot surface growth, agglomeration [1] and oxidation are elucidated by discrete element modeling (DEM) and compared to experimental data at various combustion conditions from different laboratories. The classic Rayleigh-Debye-Gans (RDG) theory is revised by coupling the discrete dipole approximation (DDA) to these DEM-derived agglomerates [2]. So by accounting for the morphology and composition of soot, the evolution of its light absorption and scattering in premixed flames is elucidated. That way both DEM-DDA and revised RDG theory can be readily used for optimizing the selectivity of fire detectors and advancing soot optical diagnostics, as well as for a more accurate estimation of the climate impact of soot.

[1] Kelesidis, G.A., Goudeli, E., Pratsinis, S.E., "Morphology and mobility diameter of carbonaceous aerosols during agglomeration and surface growth", *Carbon* 121 527-535 (2017).

[2] Kelesidis, G.A., Kholghy, M.R., Zuercher, J., Robertz, J., Allemann, M., Duric, A., Pratsinis, S.E., Light scattering from nanoparticle agglomerates, *Powder Technol.* (2019) doi.org/10.1016/j.powtec.2019.02.003.

1IM.1

Studying Coarse-Mode Aerosol Particles with Digital Holography from a UAV. MATTHEW BERG, Osku Kempainen, Jesse Laning, Ryan Mersmann, *Kansas State University*

Digital holography (DH) has proven a powerful method to study aerosol particles, particularly the relatively large coarse-mode particles. Such particles are abundant in the atmosphere in agricultural, desert, and urban environments. The accurate characterization of these particles' morphology is an important need in many scientific and applied contexts, especially to advance our understanding for how such aerosols influence the solar radiative forcing of the atmosphere. In the DH method, a particle is illuminated by an expanded laser beam and the interference pattern produced by unscattered and forward-scattered light from the particle is recorded on a sensor, i.e. a CCD. This interference pattern is the hologram, and from it, an image of the particle can be unambiguously rendered. Particles freely flowing in the atmosphere that are nominally 5 microns to several millimeters in size can be imaged this way. The relative simplicity of digital holography makes it an ideal candidate for a portable instrument for aerosol science. In this presentation, we present the design, construction, and application of such an instrument, the Holographic Aerosol-Particle Imager, or HAPI, which is mounted to an unmanned aerial vehicle (UAV). We will then discuss our initial use of HAPI to perform in situ observations of coarse-mode aerosol particles in the atmosphere.

1IM.2

Measuring Humidification Effects on Aerosol Optical Properties with a Novel Humidity Controlled Albedometer: Instrument Validation and Soot Experiments. TYLER CAPEK, Jared Lam, Christian Carrico, Claudio Mazzoleni, Allison Aiken, Timothy Onasch, Andrew Freedman, Manvendra Dubey, *Michigan Technological University*

A novel method for probing the single scattering albedo (SSA) of aerosol exposed to high relative humidity (RH) environments has been developed. A cavity attenuated phase-shift albedometer (CAPS PM_{SSA}) was integrated with a humidifier that allows us to control the RH of the sample volume. The CAPS PM_{SSA} uses a light source centered at 450nm, and the combined instrumentation was capable of measuring scattering, extinction, and relative humidity on the same sample volume. From these measurements, aerosol light absorption and SSA can be calculated. Optical enhancements were determined by taking the ratio of aerosol optical properties at high RH (85%) to aerosol optical properties at low RH (<20%). Light scattered by ammonium sulfate was enhanced by as much as 3.5 times. Likewise, the scattering and absorption of nigrosin was enhanced by as much as 1.5 and 1.2, respectively. Benchmark measurements of fresh soot confirm that they are hydrophobic, and do not take up water readily. The effects of aging of soot was studied by exposing it to a highly oxidative environment within an oxidation flow reactor. We detected a significant change in the single scattering albedo of the soot after aging, noting an increase from 0.3 to 0.4. We also investigated the change in the optical properties of soot exposed to humidified environments. In the future, we will focus our efforts on how the hygroscopic and optical properties of soot change when exposed to varying degrees of oxidation within the flow reactor.

1IM.3

Design, Characterization, and Application of a New Field-Portable Dual-Cell Multiwavelength Photoacoustic Spectrometer with Integrated Nephelometers. BENJAMIN SUMLIN, Rajan K. Chakrabarty, *Washington University in St. Louis*

We present the development, calibration, and characterization of a new field-portable Multiwavelength Integrated Photoacoustic-Nephelometer (MIPN), an in situ, real-time, contact-free instrument designed primarily for field measurements of brown carbon (BrC).

The MIPN measures light absorption and scattering at four wavelengths (405, 488, 561, and 670 nm), and uses a dual-cell design with two independently-calibrated optoacoustic cavities, each equipped with scattering, absorption, and laser power detectors. This design allows the MIPN to circumvent errors introduced by combustion by-products such as NO_x, which absorb strongly in the short visible and near-UV where BrC absorption is relevant. Typically, interfering gases are physically removed from sample streams physically with activated carbon denuders or are accounted for by frequently zeroing the instrument with aerosol-free baseline readings. Our dual-cell approach reduces all interfering phenomena (electrical and acoustic noise, absorbing gaseous species, etc.) to common-mode noise which is removed upon combining measurements. After optical analysis, the analyte is collected on a removable PTFE or quartz-fiber filter for offline analysis to further connect optical properties with physical properties (e.g., mass for mass absorption and mass scattering cross sections) and chemical properties (e.g., thermal desorption gas chromatography for molecular-level organic aerosol analysis).

We conclude with a discussion on deployment of the MIPN to the NASA/NOAA FIREX-AQ field campaign aboard the Aerodyne Mobile Laboratory, with a performance analysis and a first look at initial findings.

1IM.4

A Three-Angle Light Scattering Technique for Measuring the Single-Cycle Exhaust Soot from the Internal Combustion Engines. Pooyan Kheirkhah, Patrick Kirchen, STEVEN ROGAK, *University of British Columbia*

Soot emission from direct-injection engines is rarely steady; a few combustion cycles can dominate the total engine-out soot. Cycle-resolved measurements are currently only achievable with the costly in-cylinder optical methods. The Fast Exhaust Nephelometer (FEN) simultaneously measures the light scattering in three angles to infer the concentration and size of the PM. To develop and calibrate the FEN data processing, a series of measurements were made on steady diluted exhaust in parallel with measurements by SMPS, filter sampling and electron microscopy.

The measured FEN signal is converted to the soot concentration using a new model that incorporates the Rayleigh-Debye-Gans (RDG) and an aggregate model using recent correlations between the primary particle size and the aggregate size. The ratio of the light scattering signals measured in three angles is used to infer the average size, the geometric standard deviation, and the Mass Scattering Coefficient (MSC) of the soot aggregates. Next, the FEN was connected to a heavy-duty engine, sampling near the exhaust valve and synchronized with the engine crankshaft encoder. The response time is measured by disabling and then re-enabling the fuel injection. This high-low-high signal transition during this “skip-firing” scheme indeed shows that the instrument responds to the engine-out soot in less than 40-50 milliseconds, i.e. half of the engine cycle period over a wide range of engine speeds.

1IM.5

Investigation of Carbon Nanotube Concentrations as Elemental Carbon. PATRICK O'SHAUGHNESSY, Ralph Altmaier, Craig Holder, *University of Iowa*

In this study, we compared the gravimetric mass of carbon black and two types of multi-walled carbon nanotubes (MWCNT): small-diameter (<8 nm) and large-diameter (50-80 nm) to the mass of elemental carbon (EC) quantified by NIOSH Method 5040. A novel laboratory-based system generated an MWCNT aerosol to collect mass on quartz fiber filters ranging from 1 to 30 µg. This system utilized LABVIEW software to control solenoid valves to shut off the sampling flow rate through cyclone samplers after a desired amount of aerosol mass was deposited on a filter. The system relied on real-time concentration readings from a photometer that, in combination with a known flow rate, allowed the mass collected over time to be calculated. Both quartz fiber and PVC filters were collected for assessment by Method 5040 and gravimetric analysis, respectively. Method 5040 was conducted by a certified lab using a temperature ramping scheme suggested by NIOSH. The gravimetric and EC results were compared, and a regression model was developed for each powder type. Additionally, the limit of detection (LOD) of the NIOSH Method 5040 for each powder type was determined. The regression models had significant slopes of 0.96, 0.62, and 0.70 for carbon black, small-diameter MWCNT, and large-diameter MWCNT, respectively. The LOD determination resulted in values of 8.8, 4.5, and 8.3 µg for carbon black, small-diameter MWCNT, large-diameter MWCNT, respectively. Assuming a sample flow rate of 4.2 L/min and an 8-hour sample duration, the concentration-based LOD of NIOSH Method 5040 was 4.4, 2.2, 4.1, and 15.8 µg/m³ for carbon black, small-diameter MWCNT, and large-diameter MWCNT, respectively. These findings indicate the analysis of EC is affected by the structure and elemental content of the CNTs in such a way as to under-report the EC associated with the carbon nanotubes.

1IM.6**Evaluating the Consistency of Submicron Aerosol Mass during the Atmospheric Tomography Mission (ATom): A Focus on the Aerosol Mass Spectrometer Quantification.**

HONGYU GUO, Pedro Campuzano-Jost, Benjamin A. Nault, Douglas Day, Christina Williamson, Agnieszka Kupc, Charles Brock, Gregory Schill, Karl D. Froyd, Daniel Murphy, Eric Scheuer, Jack Dibb, Joseph Katich, Jose-Luis Jimenez, *CIRES, University of Colorado, Boulder*

The Aerodyne high-resolution time-of-flight Aerosol Mass Spectrometer (AMS) is a widely used real-time-response instrument that provides quantifiable mass and size products of non-refractory submicron chemical species. Although good agreements have been found in past field studies when intercomparing with other instruments, concerns regarding the AMS calibration have recently been discussed in the literature. This study aims to provide a critical evaluation of AMS quantification through comparisons to other well characterized and operated instruments in NASA Atmospheric Tomography Mission (ATom). These aircraft campaigns, which sampled the remote marine troposphere from 65°S to 80°N over different seasons, offer a unique opportunity to evaluate AMS quantification over a very wide range of aerosol concentrations and compositions. The NOAA particle size spectrometers (NMASS+UHSAS+LAS; measure 4nm-5µm particle number size distributions), a Particle Analysis by Laser Mass Spectrometer (PALMS; provides size-resolved particle composition when coupled with the size distributions), and a Soluble Acidic Gases and Aerosols (SAGA-IC&filters; measures inorganic ions concentrations) are included in the intercomparisons. Special attention was paid to characterize the AMS size-dependent transmission with in-field calibrations; this provides crucial context when comparing to instruments with very different size cuts. Good agreement was found between the AMS calculated volumes (including SP2 black carbon) and the submicron volume derived from the NOAA particle size spectrometers over three orders-of-magnitude concentrations (slope = 0.97 and 0.88, $r^2 = 0.93$ and 0.87, for ATom-1 and -2, respectively). A comprehensive evaluation was performed on the different sources of uncertainty and their impact on the comparison. Good agreement was also found between SAGA, PALMS, and AMS sulfate and between the PALMS apportioned organic aerosol (OA) and AMS OA. These results suggest the absence of important unknown quantification biases for AMS total mass, sulfate, and OA for the mostly aged air masses encountered in ATom.

1IM.7**Excitation Emission Matrix Spectroscopy for Analysis of Chemical Composition of Combustion Generated Particulate Matter.**

Gaurav Mahamuni, Jay Rutherford, Justin Davis, Jonathan Posner, Gregory Korshin, IGOR NOVOSSELOV, *University of Washington*

Analysis of particulate matter (PM) is important in assessing an individual's exposure to potentially harmful particles, such as aeroallergens, toxins, and emissions from combustion sources. Polycyclic aromatic hydrocarbons (PAHs) are a widespread class of environmental chemical pollutant found in combustion-generated PM. They are associated with carcinogenic and mutagenic effects. We analyze the presence of 24 PAHs having molecular weight < 302 g/mol (including the 16 PAHs recognized as priority pollutants by the EPA) in combustion-generated PM using excitation emission matrix (EEM) spectroscopy. Combustion-generated PM samples of varying PAH content were generated by combustion of ethane and ethylene fuels diluted with Argon to control the combustion temperature in an inverted gravity flame reactor (IGFR). Spectral peaks in the EEM spectra are correlated with PAH content; the data is compared with GCMS analysis on PM. A multiple linear regression model is developed using principal component regression (PCR) to predict PAH concentrations in each sample. The predictions based on the EEM spectra correlate with PAH concentrations from GCMS analysis with 34% average error. This model trained on the laboratory samples is applied to predict PAH concentrations in PM from woodsmoke and diesel exhaust samples. The approach can be used to predict relative concentration of PAHs, toxicity and carcinogenicity in combustion-generated PM.

1UA.1

Measurement of Formation Rate of Secondary Aerosols in the Urban Atmosphere Using a Dual Chamber System. SPIRO JORGA, Christos Kaltsonoudis, Aikaterini Liangou, Spyros Pandis, *Carnegie Mellon University*

The use of ambient air for studying atmospheric processes could help us bridge the gap between the idealized laboratory studies, using clean air as their starting point, and the actual atmosphere. Two identical smog chambers are used in these experiments with the first acting as a reference chamber and the second as the reaction chamber.

In this work, the dual smog chamber system was used to quantify the formation rates of secondary organic and inorganic aerosol in an urban environment (Pittsburgh, US). Ambient air was introduced in both chambers and HONO photolysis was used to produce hydroxyl radicals (OH) in the reaction chamber. The production rate of secondary organic aerosol (SOA) under typical noon-time OH concentrations ranged from 0.25-0.8 $\mu\text{g m}^{-3} \text{h}^{-1}$. The production rate of sulfate was approximately 5 times less than that of the produced SOA. Nucleation and growth of new particles was observed in the reaction chamber. The produced SOA had similar composition with the preexisting oxygenated ambient OA. The reacted amounts of the measured volatile organic compounds were able to explain 5-50% of the formed SOA in the reaction chamber. Intermediate volatility organic compounds could be responsible for the rest.

1UA.2

SOA Potential of Urban Volatile Chemical Product (VCP) Emissions Explored Using In-Situ Oxidation Flow Reactor. RISHABH SHAH, Matthew Coggon, Georgios Gkatzelis, Brian McDonald, Antonios Tasoglou, Carsten Warneke, Jessica Gilman, Heinz Huber, Allen Robinson, Albert A. Presto, *Carnegie Mellon University*

This study proves a significant pool of SOA-forming VCP emissions in urban environments. We used an oxidation flow reactor (OFR) to demonstrate that there is excess SOA potential in densely populated areas because of this pool of vapors.

Mobile sampling studies in the last 5 years have revealed ambient SOA increments in source-rich intra-urban environments (e.g., downtown). While these increments can be from rapidly-reacting combustion emissions from vehicles, McDonald et al. have shown that VCPs have comparable SOA potential. Our objectives are three-fold: 1) measure precursor levels and SOA potential in different intra-urban environments, 2) investigate contributions from vehicles, biogenics, and VCPs to observed SOA potentials, and 3) target specific VCP sources and investigate their SOA potential.

For objective #1, we performed measurements in different urban environments: e.g., urban street canyon, urban residential (UR), etc. We use mass spectrometry coupled with OFR to characterize ambient pollution levels and SOA potential. For objective #2, we use simple kinetic models to explain OFR-SOA. For model inputs, we use ambient concentrations of traditional combustion and biogenic precursors. We are able to constrain OFR-SOA in some environments using these inputs, but unable to explain ~50% of the OFR-SOA in environments with higher VCP levels (e.g., downtown street canyon, with high levels of deodorant tracer), indicating that VCPs are an additional important source of urban SOA.

For objective #3, we performed OFR measurements next to a construction site and observed correlated responses in gas-phase VCP markers and OFR-SOA. In laboratory, we oxidized specific VCP fumes (deodorant, oil-based paint) and calculated their SOA yields. We find 5 orders of magnitude variances in SOA yields of these VCP fumes, implying that further characterization of VCPs is warranted for understanding their urban SOA potential.

1UA.3**Volatility-Based Measurements of Aerosol Mixing State at an Urban Background Site in the Western United States.**

CHIRANJIVI BHATTARAI, Andrey Khlystov, *Desert Research Institute*

The volatility of organic aerosols (OA) is an important thermodynamic parameter for understanding their gas/particle partitioning, lifetime, and transport. Measurements of aerosol volatility using thermodenuders (TD) usually assume the aerosol to be internally mixed. Very little is known about the validity of this assumption. We will present measurements of ambient aerosol volatility aimed to determine aerosol mixing state at an urban background site in the western United States. The measurements took place on a roof of the Desert Research Institute in Reno, NV during July-September 2017, December-February 2018, and June-July 2018. A volatility tandem differential mobility analysis (VTDMA) with a TD residence time of 22 seconds was used to measure the aerosol volatility. Temperatures between 40°C and 200°C were scanned every 3 hours. Aerosol size distributions measured after the TD were processed to identify the main mode. The contribution (F) of the main mode to the total selected aerosol was calculated as the number concentration of the main mode divided by the total number concentration of single-charged particles selected by the VTDMA. F values below 1 indicate the presence of externally mixed particles. Our observations show that aerosols were externally mixed most of the time. The extent of the aerosol mixing state varied between winter and summer. The probability distribution of the main mode fraction (F) during summer time was negatively skewed with a mean $F=0.70$ (i.e., approximately 1/3 of the aerosol was found outside of the main mode). In winter, the distribution was positively skewed with the mean $F=0.4$. The higher degree of external mixing during winter is likely due to a stronger influence of local aerosol sources.

1UA.4**On-Road Measurement of Auto Brake and Tire Wear**

Emissions. FARZAN OROUMIYEH, Yifang Zhu, *University of California, Los Angeles*

The contribution of mobile sources to air pollution is significant, especially in urban regions. Global and national efforts in the past few decades have led to passing rules and developing technologies to diminish the mobile sources. However, what are generally referred to as mobile sources might be underestimated by limiting them to tailpipe emissions. Since previous research was mostly dedicated to the exhaust-related sources, there is a clear gap of knowledge about non-exhaust traffic sources. These others are considerable and include brake, tire and motor emissions as well as road dust.

We studied brake and tire wear particulate emissions, one of the largest contributors to non-exhaust emissions and focused on the effects of vehicles' weight on brake and tire wear emissions. Three vehicles with different weights were tested to determine the effect of the weight of the vehicles on brake and tire wear particle emissions. A full-sized SUV, a mid-sized sedan and a compact sedan were tested under an identical driving protocol on a predetermined driving route. The rationale is that since the friction force is generated by pressing the brake pads against the brake disc, more particulate matter (PM) is expected to be released from the brake lining material of heavier vehicles at a given stopping distance. First, an optimum route which had reasonable traffic load was selected. Further, the vehicles were driven on the selected route with instruments installed inside the vehicle measuring for PM_{10} and particle number concentration (PNC) and PM size distribution at two inlets: 1. brake inlet and 2. ambient inlet. The results showed an apparent increase in PM_{10} and PNC levels with an increase in vehicles' weight.

1UA.5

Lab-in-the-Field Perturbation Experiments: SOA Formation in an Ambient Matrix. JEAN RIVERA-RIOS, Adam Wright, Nga Lee Ng, *Georgia Institute of Technology*

The oxidation of volatile organic compounds (VOC) in the atmosphere leads to the formation of secondary pollutants like ozone and secondary organic aerosol (SOA). Traditional chamber experiments have been used extensively as the main tool to study SOA yields from many VOCs. However, the formation of SOA from a VOC has been shown to depend on not only the identity of the VOC but also, the oxidant, oxidant concentration, peroxy-radical fate and the concentrations of other VOCs during oxidation. Laboratory chamber studies typically push the reaction regimes to an extreme to simplify the chemistry, though recent studies have pointed to the importance of studying how different reaction parameters interact. In order to study matrix effects on SOA formation, we built an outdoor chamber in which specific VOCs are oxidized using ambient air as the matrix. A state-of-the-art instrumentation suite is employed in order to understand which variables have the strongest effect on SOA formation from VOCs and their oxidation products. In addition, the formed SOA is analyzed using positive matrix factorization in order to understand the sources of different organic aerosol factors found in ambient data. The results from these experiments can provide improved parametrizations for modeling SOA under realistic conditions.

1UA.6

Measuring Dry and Wet Deposition of Atmospheric Aerosols to Surfaces in Syracuse, NY. ALEXANDER JOHNSON, Cliff Davidson, *Syracuse University*

Dry deposition of aerosols is a major atmospheric input to the urban environment where it can degrade natural and man-made surfaces. Surrogate surfaces are frequently used to measure dry deposition fluxes, including some that are designed to minimize atmospheric turbulence and create a thin, uniform boundary layer over the surface. These characteristics can provide a measured flux that serves as a lower limit of the dry deposition onto rougher, more complex surfaces.

Wet deposition also removes aerosols from the atmosphere, and this can occur by both washout and rainout processes. While the wet deposition flux is usually measured as a time average for one precipitation event, the flux may vary within an event depending on meteorology and influences from local emissions.

Dry deposition and wet deposition were measured on the Syracuse University campus in Syracuse, NY from 2016 to 2018. The objectives were to determine ranges of dry deposition velocities of inorganic anions and to determine variations in wet deposition fluxes within individual rainstorms. Dry deposition velocities were determined by measuring the fluxes using surrogate surfaces, 1.2 meters in diameter, and by simultaneously measuring airborne concentrations. Measured dry deposition velocities were in the range of 0.6-2.5 cm/s (fluoride), 1.9-9.2 cm/s (chloride), 0.11-1.8 cm/s (sulfate), and 0.1-1.1 cm/s (nitrate). Larger deposition velocities of sulfate and chloride were obtained during the winter, possibly due to entrainment of deicing salts into the atmosphere. Fresh precipitation was collected on Jun. 4, 2017, Oct. 9, 2017, and Jul. 25, 2018 at multiple time steps during each storm. Wet deposition fluxes of sulfate, nitrate, and chloride generally decreased over time, suggesting that washout is an important process for removing contaminants. However, fluxes sometimes increased due to changes in wind direction and precipitation intensity.

1UA.7

Particle Size Distribution in a Polluted Megacity: The Delhi Aerosol Supersite Study. SHAHZAD GANI, Sahil Bhandari, Kanan Patel, Sarah Seraj, Prashant Soni, Zainab Arub, Gazala Habib, Lea Hildebrandt Ruiz, Joshua Apte, *University of Texas at Austin*

Delhi, India, routinely experiences some of the world's highest urban particulate matter concentrations. While fine particulate matter (PM_{2.5}) mass concentration in Delhi are an order of magnitude or more higher than in many western cities, the particle number (PN) concentrations are not similarly elevated. Here we report on 1.25 years of highly time resolved particle size distribution (PSD) data from the *Delhi Aerosol Supersite* study. We also supplement some of our findings using aerosol chemical composition data from our site. Details of aerosol mass and composition have already been presented in Gani et al. (2018).

While the mass concentrations between the winter and summer dropped by more than 50%, the corresponding drop for PN concentration was less than 20%. Furthermore, while it is generally assumed that ultrafine particles (UFP, $D_p < 100$ nm) make up most of the PN concentration, we observed that large number of accumulation particles—that make up most of the PM_{2.5} mass—contributed to almost half of the PN concentrations for some of the extremely polluted periods. UFP concentrations were found to be lower during periods with some of the highest mass concentrations. Calculations based on measured PSDs and coagulation theory suggest wintertime UFP concentrations suppression by a rapid coagulation sink. High wintertime particle surface area, mostly from particles in the accumulation mode, provides a plausible sink for UFP. Implications of a strong accumulation mode coagulation sink for future air quality control efforts in Delhi are that a reduction in mass concentration, especially in winter, may not produce proportional reduction in PN concentration. Long term continuous observations of PSDs from Delhi provide important insights into the role of sources and atmospheric processes that drive aerosol number concentrations.

Gani et al. (2018), Atmospheric Chemistry and Physics Discussions, <https://doi.org/10.5194/acp-2018-1066>.

2AC.1

Chemical Composition and Evaporation Rates of Secondary Organic Aerosol from Cooking Oils. MANPREET TAKHAR, Craig A. Stroud, 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. However, like many organic emissions, the physical and chemical evolution of food cooking aerosol in the atmosphere is poorly understood. Previous studies have shown significant production of secondary organic aerosol (SOA) formation, but lack the understanding of composition of SOA at molecular level. Therefore, in this work, we investigate the oxidation of cooking oil (canola, olive, beef tallow) vapors using a flow tube reactor coupled to a thermodenuder to study the composition and kinetics of SOA. The chemical analysis using a thermal desorption-gas chromatography-mass spectrometry shows that substantial fraction of SOA from cooking vapors is embedded in the unresolved complex mixture (UCM). Our results highlight that detailed speciation of UCM can be achieved based on the mass fragmentation pattern, and all the GC elutable compounds can be classified by their functional groups. Deconvoluted UCM is thus used to derive a mass-based volatility distribution. Additionally, we can use the information on polarity and volatility of the products into a two-dimensional volatility basis set to better constrain the evolution of cooking emissions. These measurements are then used as inputs into a mass transfer model to predict the evaporation rates of SOA upon heating in a thermodenuder. Moreover, heterogeneous oxidation of these cooking oil particles suggests a slower response to evaporation in a thermodenuder than unoxidized cooking oil particles. Thus, by incorporating measurements of composition and evaporation kinetics into a mass transfer model, we report 1-2 orders of magnitude decrease in mass accommodation coefficients upon heterogeneous oxidation. Similar, measurements of mass accommodation coefficients for SOA from cooking oil vapors will be presented and compared to that of heterogeneous oxidation of POA.

2AC.2

Secondary Organic Aerosol Yields of Volatile Chemical Products. SOPHIA CHARAN, Reina Buenconsejo, Yuanlong Huang, John Seinfeld, *California Institute of Technology*

Recent inventory-based analysis suggests that emissions of volatile chemical products in urban areas have become competitive with those from the transportation sector, now that emissions from motor vehicles have declined due to successful legislation. Understanding the potential for aerosol formation from these volatile chemical products is, therefore, of critical importance for predicting secondary organic aerosol and for formulating policy that will reduce aerosol exposure. A plethora of oxygenated compounds are either emitted directly into the atmosphere or emitted indoors and later escape into the outdoors. The secondary organic aerosol yields of representative compounds that have been measured in the atmosphere or are predicted to contribute significantly to the atmosphere based on inventory data are studied under conditions relevant to urban conditions: benzyl alcohol, n-butyl acetate, ethylene glycol butyl ether, and D5-siloxane. At low constant NO concentrations and 290 K, secondary organic aerosol mass yields for benzyl alcohol exceed 1.5, a yield considerably larger than previously predicted. Even at higher temperatures and different NO_x concentrations, mass yields exceed 1. Experimental and simulated environmental chamber data provide an understanding of yield under many relevant urban conditions and give insight into the effect of volatile chemical products on secondary organic aerosol.

2AC.3

Estimation of Biogenic VOC Emissions and the Corresponding Impact on Ozone and Secondary Organic Aerosol Formation in China. KAI WU, *Chengdu University of Information Technology*

Biogenic volatile organic compounds (BVOCs) play an important role in global environmental chemistry and climate. In the present work, biogenic emissions from China in 2017 were estimated based on the Model of Emissions of Gases and Aerosols from Nature (MEGAN). Based on the Weather Research and Forecasting (WRF) - Community Multiscale Air Quality (CMAQ) modeling system, the effects of BVOC emissions on ozone and secondary organic aerosol (SOA) formation were investigated. Three parallel scenarios were developed to assess the impact of BVOC emissions on China's ozone and SOA formation in July 2017. Biogenic emissions were estimated at 23.54Tg, with peak in summer and decreasing from South China to North. According to the standard CMAQ output, high ozone concentrations were mainly concentrated in the north, especially in the JJJ (Jin-Jing-Ji region), SCB (Sichuan Basin) and YRD (Yangtze River Delta). The high BVOC emissions across eastern and southwestern China increased surface ozone levels, particularly in the JJJ, YRD, SCB and central PRD (Pearl River Delta) regions, with augments of up to 47 $\mu\text{g m}^{-3}$ due to the sensitivity of VOC-limited urban areas. In addition, BVOC emissions made a large contribution to summertime SOA levels (national average of 60%).

2AC.4

Investigating the Atmospheric Age Distribution of Primary and Secondary PM during a Severe Wintertime Pollution Episode. QI YING, Hongliang Zhang, Jianlin Hu, *Texas A&M University*

High PM_{2.5} concentrations are still frequently observed in many areas in China, particularly in winter. The occurrence of these events has been shown to be highly controlled by meteorological conditions with polluted and clean days often occurring periodically. One of the unresolved questions regarding the formation of PM_{2.5} during these high pollution events is how fresh and aged emissions interact and their respective contributions to the rapid increase of primary and secondary PM. A better understanding of how freshly emitted and aged PM_{2.5} and their precursors contribute to total PM_{2.5} concentrations will allow policymakers to design cost-effective urgent emission control measures when adverse meteorological conditions are predicted.

In this study, the Community Multiscale Air Quality (CMAQ) model with a unified source- and age-resolved gases and particle representation framework is applied to investigate the January 2013 severe PM_{2.5} pollution episode in China. In the age-resolved model, the same pollutant emitted at different times (thus with different atmospheric ages) are tracked independently through the model simulations of emission, transport, transformation and removal processes so that the age distribution of the pollutant can be directly determined. To determine the age-distribution of secondary PM_{2.5} components, such as ammonium nitrate, their gas phase precursors are also modeled as age-resolved mixtures using a modified gas phase chemical mechanism. We expect to present, based on the modeling results, the hour-by-hour evolution of the age-distribution of elemental carbon (EC), organic carbon (OC), nitrate (NO_3^-), sulfate (SO_4^{2-}) and ammonium ion (NH_4^+) and the precursor gases at major urban areas as well as in regional scale during the one-month high pollution period. The correlation of atmospheric age with meteorological parameters will be study to better understand how meteorological conditions affect the accumulation and retaining of pollutants.

2AC.5

Heterogeneous Oxidation of SO₂ in Sulfate Production During Nitrate Photolysis at 300 nm: Effect of pH, Relative Humidity, Irradiation Intensity, and the Presence of Organic Compounds. Masao Gen, Ruifeng Zhang, Dan Dan Huang, Yong Jie Li, CHAK K. CHAN, *City University of Hong Kong*

Heterogeneous oxidation of SO₂ is one of the promising mechanisms to account for high loading of sulfate during severe haze periods in China. Our earlier work reported the SO₂ oxidation by OH and NO₂ produced during nitrate photolysis (*Environ. Sci. Technol. Lett.* 2019, 6, 86–91). Here, we extend that work to examine sulfate production during nitrate photolysis at 300-nm irradiation, which can additionally generate NO₂⁻ or HNO₂, N(III). Flow cell/in-situ Raman experiments showed that the reactive uptake coefficient of SO₂, γ_{SO_2} , can be expressed as $\gamma_{\text{SO}_2} = 1.64 \times p_{\text{NO}_3^-}$, the nitrate photolysis rate in the range of $(1.0 - 8.0) \times 10^{-5} \text{ M s}^{-1}$. Our kinetic model predicts that N(III) is the main contributor to the SO₂ oxidation, followed by NO₂ contribution. Furthermore, the addition of OH scavengers (e.g., glyoxal, or oxalic acid) does not suppress the sulfate production, because of the reduced N(III)-consuming reactions, and the high particle pH sustained by their presence. Our calculations illustrate that under characteristic haze conditions, the nitrate photolysis mechanism can produce sulfate at $\sim 1 \mu\text{g m}^{-3} \text{ h}^{-1}$ at pH = 4–6 and $p_{\text{NO}_3^-} = 10^{-5} \text{ M s}^{-1}$. The present study highlights the importance of nitrate photolysis in heterogeneous oxidation of SO₂ by reactive nitrogen (NO₂⁻/HNO₂ and NO₂) under atmospherically relevant actinic irradiation.

2AC.6

Impacts of Water Partitioning and Polarity of Organic Compounds on Secondary Organic Aerosols over Eastern China. JINGYI LI, Qi Ying, Jianlin Hu, Jianjun Chen, Haowen Zhang, *Nanjing University of Information Science & Technology*

Secondary organic aerosol (SOA) is a very important component of fine particulate matter (PM_{2.5}), accounting for 20–50% in urban and rural areas of China[1]. Most air quality models used an equilibrium partitioning method along with estimated saturation vapor pressure of semi-volatile organic compounds (SVOCs) to predict SOA formation. However, this method ignored partitioning of water vapor to the condensed phase as well as the polarity of SVOCs, and might result in significant underestimate of SOA[2]. Here, we used the Community Multi-scale Air Quality model (CMAQv5.0.1) to investigate the above impacts on SOA formation during winter (January) and summer (July) of 2013 over eastern China. The organic aerosol module was updated followed Pankow et al.[2] by incorporating water co-condensation and molecular structure of SVOCs. We also considered the polarity of primary organic aerosols by assuming a bulk composition of 10 surrogate species with different mass fractions following Li et al.[3]. Our model can well reproduce the mass concentration and diurnal variation of PM_{2.5} and major components. SOA concentration shows significant seasonal and spatial variation, with high levels in North China Plain (NCP), Central China and Sichuan basin areas during winter (up to 16 $\mu\text{g m}^{-3}$) and in Yangtze River Delta (YRD) during summer (up to 10 $\mu\text{g m}^{-3}$). By including water co-condensation, we see SOA increases by 20–40% in winter in Eastern China. This process leads to a relatively higher increase of SOA in summer by about 40%–80% in YRD. The polarity of SVOCs and POA exhibits negative effects on SOA formation, resulting in about 20% decrease in both summer and winter. Overall, SOA concentration varies from -10~20% to 20–40% in the high regions in winter and summer, respectively. Condensed water into the SOA portion reaches to 3 and 1.2 $\mu\text{g m}^{-3}$ in the highly concentrated areas in winter and summer, accounting for 15–30% and up to 15% of the total SOA, respectively. Such variation in both SOA and water content will further alter the physical and chemical properties of aerosols.

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2AC.7**Assessment of Model-Simulated Global Atmospheric Ammonia with Satellite Remote Sensing Measurements.**

ARSHAD NAIR, Fangqun Yu, Gan Luo, *The State University of New York at Albany*

Atmospheric ammonia, by virtue of its alkalinity and abundance, plays multiple roles in atmospheric chemistry and composition and consequently has wide-ranging effects on the environment. A myriad of effects such as increased reactive N deposition, eutrophication, acidification by nitrification, neutralization of atmospheric particles, modification of particle hygroscopicity, increasing particle uptake of acidic gases, and modification of particle mass and number concentration distributions are consequent of the presence and variability of ammonia in the atmosphere. Of recent interest is the role of ammonia in atmospheric new particle formation (nucleation), where ammonia even at the pptv levels has been shown to radically increase rates of inorganic nucleation as well as play a role in organic nucleation. This has implications for aerosol radiative forcing, which remains the largest source of uncertainty in climate change modeling. These aspects combined with the increasing trend of gas-phase ammonia across most of the globe motivate the current assessment of multi-year GEOS-Chem (a 3D global atmospheric chemistry model) simulated ammonia with satellite remote sensing measurements, which provide the advantage of a continuous global scope over in situ measurements. Model simulated ammonia is in good spatial agreement with satellite observations, with co-located ammonia source regions and hotspots. While simulated magnitude of column ammonia is generally underestimated (Mean Fractional Bias (MFB): $-1.4 \pm 0.6(1\sigma)$), there is a marked contrast between land (MFB: -1.0 ± 0.7) and ocean (MFB: -1.5 ± 0.5). Over ammonia source regions, this underestimation is less pronounced (MFB: -0.7 ± 0.6). We will discuss the model-observation deviations, reasons for these deviations, limitations of in-model processes and satellite data, avenues for improvement, and the consequent implications especially for atmospheric new particle formation.

2AC.8**Acid-base Reactive Uptake of Dimethylamine and Nitric Acid onto Nanoparticles: Cluster Simulations and Nanoparticle Composition Measurements.**

SABRINA CHEE, Nanna Myllys, Kelley Barsanti, Bryan Wong, James Smith, *University of California, Irvine*

Nanoparticle composition measurements and cluster simulations of particle formation and growth via reactive uptake of nitric acid (HNO₃) and dimethylamine (DMA) have been investigated. A flow tube reactor with adjustable reaction time was used to study particle formation from these species under both dry and humid conditions. A Thermal Desorption Chemical Ionization Mass Spectrometer was used to measure size-resolved nanoparticle composition from 9 – 30 nm in diameter, and those results were compared with simulations of clusters up to 1 nm in size to probe the mechanism of reactive uptake. Particles were produced readily in both dry and humid (55% relative humidity, RH) conditions. Humid conditions did not significantly increase particle number concentration but increased the geometric mean diameter of the particle number-size distribution. HNO₃-DMA particle composition measurements show that the acid:base ratio remains neutral (1:1) in both RH conditions at all studied sizes. Additionally, cluster simulations strongly suggest that a 1:1 acid-base ratio is the most stable cluster growth pathway due to over 7 orders of magnitude lower evaporation rates compared to other cluster combinations. These results contrast with composition measurements of particles made from sulfuric acid (H₂SO₄) and DMA as well as NH₃, and it is likely that these compositional differences between H₂SO₄-DMA particles and the particles in this study are due to the components' volatility. Whereas HNO₃ and DMA must neutralize each other to remain in the particle phase, H₂SO₄ has a low enough volatility that it can contribute to nanoparticle growth without reactive uptake and thus particles are likely to be more acidic. Implications of these observations on ambient nanoparticle composition are discussed.

2AC.10

Viscosity of SOA Formed from Stressed and Healthy Pine Tree Emissions under Varying Oxidation Levels. NATALIE SMITH, Jesse Crescenzo, Anusha P.S. Hettiyadura, Ying Li, Celia Faiola, Alexander Laskin, Allan Bertram, Manabu Shiraiwa, Sergey Nizkorodov, *University of California, Irvine*

Secondary organic aerosols (SOA) derived from plant emissions make up a major fraction of total SOA in the atmosphere. When plants are stressed under herbivory their volatile organic compound (VOC) emission profiles change in both quantity and types of compounds being emitted. For example, when pine trees are stressed due to an aphid-herbivory attack they emit more sesquiterpenes, which can lead to the formation of different SOA when compared to SOA formed from healthy plant emissions. The chemical composition of SOA determines particle viscosity, which in turn can impact photochemical processing of particles, their ability to act as cloud condensation and ice nuclei, and lifetimes of particulate pollutants in the atmosphere. This study investigates how the different chemical composition of SOA generated from emissions of healthy vs. stressed plants, and then aged by different level of OH exposure, affects particle viscosity. Aerosols are generated in an oxidation flow reactor using a mixture of VOCs to represent either stressed or healthy pine trees. In the oxidation flow reactor, the VOCs are oxidized under low, medium, or high levels of hydroxyl radical with particle loading adjusted to be below 100 mg/m³ (this procedure will be repeated for real pine tree emissions under healthy conditions and stressed conditions when exposed to aphids). Detailed information on particle molecular composition is gained through Nano-Desorption Electro Spray Ionization –High Resolution Mass Spectrometry. The observed molecular formulas are used to predict the viscosity as a function of relative humidity using the parameterization developed by Shiraiwa et al. The predictions from the Shiraiwa model are compared to the experimentally determined viscosity values measured with the poke-flow method. The information attained from this study will help generalize the effects of viscosity so current atmospheric models can be improved upon and thus better inform public policy.

2AC.11

Investigating Brown Carbon Formation in Ambient Aerosols Undergoing Drying. VIKRAM PRATAP, Michael Battaglia Jr., Annmarie Carlton, Christopher Hennigan, *University of Maryland, Baltimore County*

A number of recent laboratory studies observed the formation of brown carbon (BrC) in aerosols undergoing drying. Since ambient particles undergo natural cycles of drying and water uptake each day, this process may contribute substantially to the atmospheric BrC budget. However, BrC formation in ambient particles undergoing drying has not been observed. In this work, we investigated drying-induced BrC formation in ambient particles sampled at Baltimore, MD. Our study included observations during both summer and winter: results from these periods are contrasted. During summer, we find no evidence of BrC formation in particles dried to ~ 40% relative humidity (RH). Diurnal variation suggests particulate water-soluble organic carbon (WSOC_p) and BrC concentrations were strongly influenced by SOA formed during the daytime. The observations are consistent across several weeks of measurements, which included a wide range of temperatures, RH levels, and aerosol loadings. Results from the wintertime data also suggest no BrC formation occurred during particle drying. The low concentration of BrC precursor compounds in ambient particles likely explains the lack of measurable BrC formation in a single drying cycle induced by our experimental setup. This process may still represent an important source of light-absorbing organic aerosols if multiple humidification-drying cycles contribute minor amounts of BrC leading to gradual buildup, or in evaporating clouds and fog, a regime our study did not investigate.

2AC.12

Effect of Relative Humidity on Secondary Brown Carbon Formation in Evaporating Droplets. NETHMI KASTHURIARACHCHI, Laura-Helena Rivellini, Xi Chen, Yongjie Li, Alex Lee, *National University of Singapore*

Secondary organic aerosols (SOA) formed via aqueous-phase reactions have been identified as a prominent pathway for brown carbon (BrC) formation. Water-soluble volatile organic compounds such as glyoxal and methylglyoxal produce BrC from reactions with inorganic and organic reduced-nitrogen species in bulk solutions on the order of days. Such reactions can be substantially accelerated upon droplet evaporation, where BrC is formed on the order of seconds. However, despite aerosols being exposed to a wide range of relative humidity (RH) throughout their atmospheric lifetime, BrC formation in response to surrounding RH remains poorly understood.

This is the first study to investigate BrC formation in evaporating droplets and to quantify their mass absorption coefficient (MAC) as a function of RH through reactions of glyoxal and methylglyoxal with ammonium sulfate (AS) or glycine. The general variations of MAC at respective peak wavelengths were similar for all systems; low MAC was observed in the bulk solutions, but MAC steadily increased and peaked at ~55-65% RH and declined towards lower RH (~30%). The initial increase of MAC is attributed to the acceleration of reactions promoted by the highly concentrated solute environment, while further drying may have led to evaporative loss of reactants and reduced mobility of molecules undergoing aqueous reactions. Hygroscopic studies revealed that phase-transition may be related to the observed variation. Furthermore, organo-nitrogen compounds can have substantial contribution to light absorption in these chemical systems. Aerosol mass spectrometric measurements showed vastly different variations in N:C ratio as a function of RH for the AS and glycine systems, indicating the potential difference of their underlying chemistry and/or product volatilities. Overall, our results highlight the significance of investigating BrC formation under various RH conditions. The effects of RH on BrC formation in complex SOA mixtures will be further discussed.

2AC.13

Size-resolved Chemical Composition of Sub-40 nm Particles during New Particle Formation and Growth Events in Beijing. XIAOXIAO LI, Yuyang Li, Chao Yan, Sabrina Chee, Jiming Hao, James Smith, Jingkun Jiang, *Tsinghua University*

The rapid growth of newly formed particles increases atmospheric CCN concentration. Direct measurement of sub-40 nm particle chemical composition helps to study the role of various physical and chemical mechanisms during atmospheric particle growth events. We carried out a field campaign in Beijing during the spring and summer of 2019 to study the growth of newly formed particles. A thermal desorption chemical ionization inlet coupled with high-resolution time-of-flight mass analyzer (TD-CI-HTOF), with O_2^- and $C_5H_{10}NO^+$ as the reagent ions, was used to measure size-resolved chemical composition (sulfate, nitrate, ammonia, amine, and organics) of sub-40 nm particles. A CI-LTOF, with NO_3^- as the reagent ion, was used to measure gas precursors including H_2SO_4 and highly-oxygenated molecules (HOMs) that are potentially relevant to particle growth. Electrical mobility size spectrometers were used to measure aerosol size distributions from ~1 nm to 10 μm . Aerosol growth model was used to evaluate the role of condensational growth contributed by gas phase H_2SO_4 and HOMs. The modeled growth rate was compared to that directly estimated from the measured particle size distributions. Size-resolved acid/base ratio, organics/inorganics ratio, and organic O/C, H/C ratio measured by TD-CI-HTOF were compared with those predicted by aerosol growth model. The relative importance of condensational growth and other mechanisms were explored.

2AC.17

The Effect of Particle Physicochemical Properties on the Uptake of Semi-volatile and Intermediate-volatility Organic Molecules. YIMING QIN, Junfeng Wang, Yali Lei, Jianhuai Ye, Scot T. Martin, *Harvard University*

Semi-volatile and intermediate-volatility organic compounds (S/IVOCs) play an essential role in the production of atmospheric particulate matter (PM), its chemical aging, and composition changes in preexisting particles. Mass transfer of S/IVOCs to preexisting particles is known to be sensitive to the physicochemical of the particles yet the detail mechanisms remain poorly understood. To address this issue, we combine experimental observation and theoretical model to investigate the effect of particle physical state and acidity on the uptake of S/IVOCs of different functional groups. In the controlled experiment, S/IVOCs were mixed with liquid, solid, partial neutralized to fully neutralized sulfate particles in a continuously mixed flow reactor. Solid sulfate particles represent one limit where uptake is limited to surface deposition (i.e., effectively infinitely small diffusion coefficient into the interior). Liquid sulfate particles took up significant amounts of S/IVOCs depending on the aerosol liquid water content, the extent of neutralization and the mixing time. An updated kinetic and thermodynamic model is being developed to estimate the gas-particle exchange of S/IVOCs to PM host composition under environmentally relevant conditions.

2AC.18

Temporal Distribution of Short-Lived Climate Forcers, Atmospheric Processes, and Sources at IGP-CARE Site in India for Two Years in-situ Measurements. RAVI KANT PATHAK, Harsh Raj Mishra, Bhilok Chand, Jai Prakash, Mattias Hallquist, Gazala Habib, Johan Boman, Håkan Pleijel, *University of Gothenburg, Sweden*

Short-lived climate forcers (SLCF) including black carbon (BC), light absorbing organic aerosol (OA): referred as brown carbon (BrC), atmospheric brown clouds (ABC), sulfate and nitrate aerosol; tropospheric ozone (O₃), carbon monoxide (CO), and nitrogen oxides (NO_x), affect the global climate and human health¹⁻³ and their atmospheric chemistry can also play an important role in Indo Gangetic Plains (IGP) region in India, where 750 million people burn biomass for cooking, heating and agricultural purposes. This study aims to understand the variability of the SLCFs – BC, BrC and O₃, by long term in-situ measurements to elucidate the relevant processes involved in rural India. Here, we will present the results from January 2017 to December 2018 measurements at the IGP-CARE (IGP-Centre for Air Research and Education). The IGP-CARE site is a representative rural location (25. 48' 55.5" N; 79o 55' 07.5" E) at the middle outflow of IGP. BC and BrC were measured by BC Monitor (BC 1050 series, Met One Instruments, Inc.) on quartz filter tape at two wavelengths (375nm; 880nm). Gaseous species including O₃, CO, and NO_x along with the meteorological parameters (e.g. WS, WD, RH, T, precipitation etc.) were measured simultaneously using standard commercial instruments. Molecular speciation of organic aerosol species was performed offline using HR-TOF-CIMS (High Resolution Time of Flight Chemical Ionization Mass Spectrometry) and particle collected on the filters.

The results provided insight that temporal distribution the pollution episodes in the winters at the IGP-CARE site were of regional and super-regional scale. A very interesting diurnal variations of BrC/BC ratio was observed. It sharply decreased during day hours and increased in night, which indicates bleaching of BrC. The bleaching of BrC is thought to be affected by temperature, photo- and/or radical chemistry. Chemistry of BrC bleaching is explored and will be presented.

2AC.19

Temperature Effects on Sulfuric Acid Aerosol Nucleation and Growth: Initial Results from the TANGENT Study. LEE TISZENKEL, Chris Stangl, Justin Krasnomowitz, Qi Ouyang, Michael J. Apsokardu, Murray Johnston, Shanhu Lee, *University of Alabama Huntsville*

New particle formation (NPF) accounts for much of the aerosol size distribution that is observed in the ambient atmosphere. The NPF process consists of two steps: nucleation and subsequent growth. At present, chemical and physical mechanisms that govern these two processes are not well understood. Here, we report initial results obtained from the TANGENT (Tandem Aerosol Nucleation and Growth Environment Tube) experiments. The TANGENT apparatus enables us to study these two processes independently with a suite of instrumentation that allows for monitoring of particle size distributions from 1 nm to 100 nm both in the temperature-controlled nucleation region as well as at the end of a separate growth region. The present study focuses on the effects of temperature on sulfuric acid nucleation and further growth. Our results show that lower temperatures enhance both the nucleation and growth rate. However, under temperatures below 268 K the effects of temperature on the nucleation rate become less significant and the nucleation rate becomes less dependent on RH, indicating that particle formation takes place via barrierless nucleation at lower temperatures. We also examined the growth of newly formed particles under differing temperature conditions for nucleation and further growth. Our results show that newly nucleated clusters formed at low temperatures can indeed survive evaporation and grow in a warmer environment in the presence of SO₂ and ozone. These results also imply that some heterogeneous reactions involving nanoparticles affect nucleation and growth of newly formed particles.

2AC.20

Laboratory Studies of the Photolysis of Particulate Nitrate. QING YE, Qianwen Shi, Jennifer G. Murphy, Jesse Kroll, *Massachusetts Institute of Technology*

Recent studies have suggested that the photolysis of particulate nitrate can recycle NO_x rapidly enough to significantly affect the NO_x budget in areas far from NO_x sources. However, reported nitrate photolysis rates differ by orders of magnitude, and experimental measurements of nitrate photolysis have mostly been conducted using indirect methods (e.g. collecting particles on substrates). In this work, we perform controlled laboratory experiments to better constrain the photolysis rate and products of suspended submicron nitrate-containing particles under various atmospherically-relevant wavelengths and relative humidities. A suite of instruments that measure particle-phase nitrates and gas-phase NO_x and NO_y species in real time are used to understand the atmospheric fate of N-containing species following photolysis. The systems studied include inorganic nitrates (NaNO₃, NH₄NO₃) as well as organic nitrates derived from terpene oxidation under high-NO_x conditions. Results can be used to inform global models of nitrate chemistry, and are aimed at improving our understanding of the lifecycles of reactive nitrogen species and their implications for global climate and air quality.

2AC.21

Terpene Emissions and Their Oxidation Products in Forest Areas: Insight from Vocus PTR-TOF Measurements. HAIYAN LI, Pekka Rantala, Kaspar Daellenbach, Jordan Krechmer, Douglas Worsnop, Markku Kulmala, Matthieu Riva, Mikael Ehn, Federico Bianchi, *University of Helsinki*

On the global scale, biogenic volatile organic compounds (BVOCs) contribute a large fraction of secondary organic aerosol production. However, due to the complex characterization of organic mixtures, an incomplete understanding of BVOCs oxidation still exists and leads to large uncertainties in quantitative estimates of air quality and climate effects of atmospheric aerosol. In this study, the recently developed Vocus PTR-TOF (proton transfer reaction time-of-flight mass spectrometry) was deployed at the SMEAR II station (Station For Measuring Forest Ecosystem-Atmosphere Relations), a boreal forest site in southern Finland. This station is known with high terpene emissions, thus providing a good opportunity to investigate the characterization of terpenes and their oxidation products. This work will give an overview of the ion molecules observed by Vocus PTR-TOF, and compare the results with those from the chamber study of α -pinene ozonolysis in the presence of NO_x and the ambient observations in Landes forest in southwestern France. With a new chemical ionization source and focusing ion-molecule reactor, the Vocus PTR-TOF detected not only terpene precursors but also various terpene oxidation products and intermediates due to improved measurement precision and detection limits. The ambient behaviours of different terpenes and their oxidation products, including both non-nitrate organic compounds and organic nitrates, will be characterized in detail at SMEAR II station, and compared with observations in Landes forest. The comparison among different environments will provide more insights into the complicated terpene chemistry.

2AD.1

An Alternative Model for Testing of Acute Respiratory Local Toxic and Physiological Effects Based on in Vitro and Isolated Perfused Lung Technologies. DETLEF RITTER, Jan Knebel, Sabrina Wilde, Tanja Hansen, Katharina Schwarz, *Fraunhofer ITEM, Germany*

Due to the demand for further developments of predictive, robust alternative models in inhalation toxicology, a combined in vitro / ex vivo model was set up to cover both local acute toxic effects and respiratory physiological effects from inhalable powders.

The in vitro and ex vivo approaches are based on an air-lifted interface (ALI) cell culture model and an isolated perfused rat lung (IPL) model including exposure to highly concentrated aerosols generated from small amounts of micronized powders.

The in vitro inhalation model included a human lung alveolar epithelial cell model (A549), an optimized exposure device (P.R.I.T.® ExpoCube®), determination of cytotoxicity and dosimetry considerations. During inhalation testing with the isolated perfused lung, physiological respiratory parameters such as tidal volume, dynamic lung compliance and relative increase in lung weight were determined, offering insight into acute physiological respiratory effects.

Four commercial fungicides and sodium-dodecyl sulfate (SDS) were used as test items and positive control for acute local lung toxicity. Small amounts of testing materials of less than 500 mg were needed in each model to establish complete dose-response curves. EC50-values from in vitro testing were correlated to LD50 values from acute rat inhalation in vivo testing and showed good predictivity. Similarly, exposure to the test items as well as to the positive control SDS resulted in formation of oedema and for SDS also in acute decrease of lung function parameters in the IPL model as a measure for acute respiratory toxicity. Hence, the inhalation effects from toxic fungicides could primarily be assigned to cell toxicity. In summary, the complementary in vitro / ex vivo model appeared very promising to investigate both acute local lung toxicity and respiratory physiological effects from inhalation of bulk powder material using only small amounts of material with short study times and meaningful predictivity.

2AD.2

Mimicking the Human Respiratory System: Online In Vitro Cell Exposure and Toxicity Assessment of Welding Fume Aerosol. RYAN WARD, Trevor Tilly, Sarah Robinson, Arantzazu Eiguren Fernandez, Jun Wang, Tara Sabo-Attwood, Chang-Yu Wu, *University of Florida*

The use of air-liquid interface (ALI) cell culture exposures are of rising interest due to their potential for improving in vitro toxicological studies. A novel ALI system, the Dosimetric Aerosol In Vitro Inhalation Device (DAVID), has been demonstrated for effective particle deposition to ALI cell culture. Additionally, this system uses water-based condensation to enhance particle deposition, which is bioinspired by the human respiratory system. In this study, welding fumes, a well-established source of airborne particle toxicity, were used to demonstrate the ability of DAVID to generate unique, dose-dependent toxic responses between two welding conditions: a baseline welding fume and an amorphous silica-coated welding fume created through the addition of tetramethylsilane (TMS) to the shielding gas flow for decreased toxicity. With the lactate dehydrogenase assay, the cells cultured at the ALI had over 50% decrease in viability in just eight minutes of exposure to baseline welding fumes, while the cells exposed to TMS-coated welding fumes had just a 10% decrease in viability over the same exposure time and exposure dose of 275 $\mu\text{g}/\text{cm}^2$. DAVID delivers a substantial dose in minutes making it beneficial over previous systems which require hours of exposure. These results demonstrate a proof-of-concept for the effectiveness of TMS to reduce toxicity to cell culture, and also the ability of DAVID to generate a distinct toxicological response for the aerosol being exposed. The submerged cell culture toxicity analysis was also performed for comparison and showed a relative decrease in toxicity after TMS was added to the shielding gas, but this trend was only observable after doses greater than 100 $\mu\text{g}/\text{mL}$. The difference between the ALI and submerged cell culture results indicates the sensitivity of the ALI cell culture approach in comparison to the submerged cell culture. Further work to quantify uncertainties in the prediction of deposited dose through DAVID is recommended.

2AD.3

Applications of the Multi-angle Imager for Aerosols (MAIA) for Air Quality and Health: Connecting Particle Mixtures to Human Health. ABIGAIL NASTAN, Sina Hasheminassab, Kristal Verhulst, David Diner, Feng Xu, Olga Kalashnikova, Michael Garay, Bart Ostro, *Jet Propulsion Laboratory*

The NASA Multi-Angle Imager for Aerosols (MAIA) investigation seeks to extend our current understanding of the impact of the amount and composition of outdoor, airborne fine particulate matter on adverse health outcomes. The MAIA satellite instrument, in development at the Jet Propulsion Laboratory and planned for launch in mid-2022, will collect multiangular, multispectral, and polarimetric measurements over a set of globally distributed targets. Retrievals of aerosol properties will be combined with ground-based air quality monitor data and chemical transport modeling to produce 1-km gridded data products of daily-averaged PM_{10} and $\text{PM}_{2.5}$ mass, and the fractional abundances of sulfate, nitrate, organic carbon, elemental carbon, and dust making up $\text{PM}_{2.5}$ mixtures. These will be freely available, and the air quality and public health communities are invited to use them. The MAIA Science Team includes epidemiologists who will use these data products in studies aimed at associating health risk with specific particle types; researchers are encouraged to also consider related projects such as source apportionment.

Characteristics of the candidate target areas, the planned MAIA data products, and opportunities for collaboration with epidemiologists and other interested stakeholders will be discussed. MAIA's Primary Target Areas (PTAs) comprise the main focus of the MAIA investigation, while Secondary Target Areas (STAs) include areas of interest for air quality, climate, and other applications. The target areas represent populous urban areas with available ground monitor data, situated geographically where they can be observed frequently from MAIA's near-polar orbit, and without persistent cloud cover. In addition, the MAIA team has selected the candidate PTAs to represent a range of typical PM concentrations and compositions. Some PTA candidates were chosen to represent areas where health impacts are significant and a lack of significant ground-based monitoring has limited the number of studies conducted to date.

2AD.4

A Comprehensive Assessment of the Spatiotemporal Variability of Oxidative Potential of Ambient PM_{2.5} in Midwest U.S. using a Semi-Automated Multi-Endpoint ROS-Activity Analyzer (SAMERA). HAORAN YU, Joseph Puthussery, Yixiang Wang, Vishal Verma, *University of Illinois Urbana-Champaign*

The capability of ambient fine particles to generate reactive oxygen species (ROS) (referred to as the oxidative potential or OP) has been associated with myriad health effects on human. Many chemical assay protocols have been developed to simulate different mechanisms of PM_{2.5}-catalyzed ROS generation, yet no consensus has been reached in selecting the most relevant method. In this study, a semi-automated multi-endpoint ROS-activity analyzer (SAMERA), which integrates five commonly used OP assay endpoints [ascorbic acid (AA) and glutathione (GSH) consumption in surrogate lung fluid (SLF), dithiothreitol (DTT) consumption and •OH generation in SLF and DTT] has been developed and employed in a large-scale spatial sampling. We collected 72 h integrated ambient PM_{2.5} samples from four urban sites and a rural site in Midwest U.S. region (including Illinois, Missouri and Indiana states) in May 2018 – May 2019, as a part of the Midwest Campaign (MWC) project. We are currently analyzing the OP of these ambient PM_{2.5} filter samples by SAMERA system, to assess the seasonal and spatial variabilities of OP compared to PM_{2.5} mass. We will also analyze these filters for the various chemical components such as HULIS, organic and elemental carbon, metals and inorganic ions. The correlations among different OP endpoints and with the chemical composition in different seasons and sites will also be presented. This study accommodates the most comprehensive list of the OP indices in a single investigation, which will be applied on a very large number of PM samples collected from an extensive spatial scale.

2AD.5

New Approach for Source Apportionment of Toxicity by Atmospheric Organic Aerosols. AKIHIRO FUSHIMI, Daisuke Nakajima, Akiko Furuyama, Go Suzuki, Tomohiro Ito, Kei Sato, Yuji Fujitani, Yoshinori Kondo, Akinori Takami, *National Institute for Environmental Studies, Japan*

Fine particulate matter (PM_{2.5}) in the atmosphere is of high priority for air quality management efforts due to observed associations with adverse effects on human health. To examine countermeasures against PM_{2.5} emission, origins of PM_{2.5} should be elucidated. On the other hand, toxicity per PM mass can remarkably differ among emission sources or atmospheres in different places. Therefore, it is better to understand source contributions not only to PM_{2.5} mass but also to PM_{2.5} toxicity. In this study, we have proposed a new approach to estimate source contributions to various kinds of toxicities by atmospheric organic aerosols (OA), using chemical mass balance model and toxicity data. To see how this approach works, we performed the following studies.

First, we chose four kinds of sources (i.e. secondary organic aerosols: SOA, automobiles, open burning of biomass, and cooking) as possible important OA sources for source apportionment. Then we conducted source testing and collected PM_{2.5} samples from these sources. We also collected ambient PM_{2.5} samples in different places (e.g. Ryogoku, Tokyo as an urban site; northern foot of Mt. Fuji as a forest site; and Hedo, Okinawa as a remote site in summer) for evaluating our approach. The chemical composition (i.e. elemental carbon, organic carbon: OC, ionic species, elements, and organic compounds) of the PM_{2.5} samples were measured. Cytotoxicity and cellular responses to the samples, including oxidative stress (measured with gene expression of heme oxygenase-1 and reporter gene assay for Nrf2), DNA-damage (measured with *umu* test), inflammation (measured with gene expression of interleukin-8), and aryl hydrocarbon receptor agonist activity, were also quantified.

We have done the chemical analysis and the in-vitro bioassays for some source and ambient samples. All kinds of cellular responses per OC of diesel exhaust particle samples were 3–10 times or larger than the biogenic SOA samples. Among the above-mentioned ambient PM_{2.5} samples collected, the urban site samples had the largest cellular responses per OC followed by the forest site samples. The remote site samples consistently showed the weakest cellular responses. In the presentation, we will show the additional results.

2AD.6**Using a Quartz Crystal Microbalance to Measure the Mass Concentration of Combustion Particle Suspensions.**

KAMALJEET KAUR, Isabel C. Jaramillo, Hamid Ghandehari, Chris Reilly, Robert Paine, Kerry Kelly, *University of Utah*

The majority of in vitro and in vivo instillation studies require generating combustion particle suspensions prior to exposure, and the mass concentration of these suspensions is critical to determining the delivered dose. However, the hydrophobic nature of combustion particles poses difficulties in getting a well-suspended mixture in DI water and an accurate estimate of delivered dose. This study explored the applicability of a quartz crystal microbalance (QCM) in estimating the mass concentration of combustion particle suspensions. It compared the QCM mass concentration to that estimated by placing a known mass of combustion particles in DI water. Standard reference diesel particles and flame-generated particles were used for the method development and calibration of QCM. The effect of suspension drop size on QCM measurements was also evaluated. For small drop volumes (0.5 μL) and constant temperatures, the QCM provides accurate and precise estimates of mass concentration for reference diesel PM ($\pm 0.7\%$) and flame-generated combustion particles ($\pm 7\%$). The application of QCM can be further extended to estimate the total mass of dissolved organic species and particle mass lost to the walls of vials.

2AD.7**Characterization of Air-Liquid-Interface (ALI) in vitro Exposure Systems for E-vapor Aerosol Applications.**

JINGJIE ZHANG, Michael Oldham, Russell Wolz, Pavel Kosachevsky, Utkarsh Doshi, I. Gene Gilman, Kyeonghee Lee, *Altria Client Services LLC*

Direct delivery of aerosol or vapor to the apical surface of cells (ALI) allows clinically relevant exposure for in vitro toxicological evaluation of inhalable chemicals. However, dose assessment in the ALI exposure system remains a challenge, especially for evolving aerosols such as e-vapor. In this study, we quantitatively characterized the aerosol delivery in commercially available ALI in vitro exposure systems (Vitrocell® Ames 48 (Ames 48) and Vitrocell® 24/48 (VC 24/48)) for e-vapor applications.

A cig-a-like test cartridge filled with a prototype e-liquid containing propylene glycol, glycerin, nicotine and water was used to generate e-vapor aerosols using a Vitrocell® 1/7 puffing machine. Aerosol size distribution, mass deposition, and effective delivery to the exposure inserts (i.e. the petri dish in the Ames 48 or transwells in the VC 24/48) were measured for both Ames 48 and VC 24/48 systems with the regular aerosol delivering method per manufacturer's instructions. Results showed that 1) the MMAD of the delivered aerosol was below 1.5 μm with the GSD between 1.8 to 2.1 as measured with a cascade impactor; 2) aerosol delivery in the exposure inserts increased linearly with the puff number; and 3) there was about 30% loss of aerosol mass in the aerosol transportation path prior to entry into the exposure system. To minimize aerosol loss, we revised the aerosol delivering method by shortening the transportation path and showed that 1) the aerosol loss prior to the exposure system was reduced to $\sim 10\%$; 2) aerosol delivery to the exposure inserts was increased up to 3 fold compared to that of the regular delivery method. Aerosol chemistry was also analyzed. The methods developed in this study can be applied to standardize the ALI aerosol characterization of e-vapor products.

2AD.8

Exposure to Portable Gasoline Generator Emissions and Its Effects on Renal Function and Lung Histology using Rat Model. GODSON ANA, Emmanuel Obansa, *University of Ibadan*

Previous studies had examined gasoline generator emissions (GGEs) profile but information about their sub-acute and non-fatal toxicological effects is inadequate. This study assessed the levels of GGEs and their effects on renal indices and lung histopathological conditions.

Three experimental groups of eight rats each were subjected to 5, 10 and 15 minutes exposure to GGEs per day for twenty-one days between the hours of 4 and 5pm with the fourth group not being exposed. Levels of CO, NO₂, VOC and PM_{2.5} in the emission chamber were recorded simultaneously using the appropriate air samplers and compared with guideline limits. Twelve hours after completion of exposure monitoring, blood was collected for renal function tests via ocular puncture while lung tissues were collected after the animals were sacrificed. Hematoxyline and Eosin (H & E) method was used to examine the lung tissues. Data collected were analysed using ANOVA and statistical significance was set at $p = 0.05$.

One-hour TWA levels of CO, NO₂, VOC and PM_{2.5} recorded in the chamber were 968ppm, 2.43ppm, 100ppm and 17.6 mg/m³ respectively. Blood urea nitrogen and creatinine tests showed significant ($p < 0.05$) increases in the test groups compared with controls. Histopathological examinations showed lesions like alveolar edema, infiltration of inflammatory cells and thickening of the alveolar interstitium in lung tissues of the exposed rats.

Exposure to GGEs at non-lethal concentrations chronically portends deleterious effects on renal and pulmonary systems. There is a need to minimise exposure and to embrace cleaner fuels.

2AE.1

Applying Mass Spectral Techniques to Identify the Chemical Composition of e-Cigarette Smoke and Its Surrogates: Implications for Source Apportionment. YUE ZHANG, Sarah Suda Petters, Manjula Canagaratna, Jonathan Thornburg, Jason Surratt, *University of North Carolina at Chapel Hill*

Electronic cigarettes (e-cigarettes), a new type of cigarette that vaporizes a mix of chemicals (so called e-liquids, which includes nicotine, is getting increasingly popular among the general population (especially in adolescents) due to its claim of being safer than traditional cigarettes. As a result, it is important to identify the chemical constituents that make up this aerosol mixture to aid in exposure assessments. This study systematically examines the chemical properties of e-liquids from an aerosol atomizer and a commercially available e-cigarette device with a range of selected compositions and operation settings. Results show that despite e-liquids consisting of primarily propylene glycol (PG) and glycerol (VG), most of the aerosol composition is dominated by VG due to its lower vapor pressure. Positive matrix factorization (PMF) of aerosol mass spectral data was successfully applied to the e-cigarette smoke with varying compositions in order to separate the mass contributions of pure PG and VG to the generated aerosols. Tracers ions with mass-to charge ratios (m/z) at 27, 41, 55, and 70 were characteristic of aerosols containing pure PG, while ions at m/z 15, 31, 43, and 61 were associated with pure VG-derived aerosols. The aerosol mass spectra of pure PG and VG were also combined with the multilinear engine (ME-2) in order to conduct source apportionment of PG and VG in both the atomized aerosols and e-cigarette smoke. Results were compared with aerosols collected on filters that were analyzed by liquid chromatography interfaced to electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (RPLC/ESI-HR-QTOFMS). VG was found to be the main component of aerosols vaporized from most e-liquids. This study establishes a source appointment method that can used to identify e-cigarette smoke and the relative contributions of pure PG- and VG-derived aerosols, and thus, can be used for air monitoring, tobacco control, and health improvement.

2AE.3

Exposure to Particulate Matter at an Outdoor Marijuana Consuming Event. TONGKE ZHAO, Kai-Chung Cheng, Wayne Ott, Lance Wallace, Lynn M. Hildemann, *Stanford University*

On April 20th of each year, marijuana enthusiasts gather at open public places to celebrate and consume marijuana together starting exactly at 4:20 pm. High levels of secondhand exposure to marijuana emissions may occur at these events, as well as at other special events (e.g. rock concerts) which allow marijuana smoking. To assess secondhand exposure to marijuana, we monitored airborne particle concentrations at outdoor marijuana consuming event on April 20th, where ~1500 people gathered in a ~20 ×50 m meadow.

PM_{2.5} concentrations and ultrafine particle concentrations were measured by two optical particle monitors (SidePak AM510, TSI Inc., Shoreview, MN) and a condensation particle counter (CPC 3007, TSI Inc., Shoreview, MN), respectively, before, during, and after the event, which lasted about 13 minutes. A calibration factor was applied to the SidePak data to estimate PM_{2.5} mass.

The background before the event was only 1.5 µg/m³ (SD=1.4 µg/m³). During the event's active-consuming period, between 4:20 and 4:33 pm, the mean PM_{2.5} concentrations were 300 µg/m³ (SD=408 µg/m³) in the crowded meadow. The maximum 1-second peak PM_{2.5} concentration was >3000 µg/m³. In an unoccupied space away from the meadow, a peak PM_{2.5} concentration of ~600 µg/m³ was measured when a single active marijuana smoker passed nearby.

The mean particle number concentration during the event's active-consuming period was 5.6×10⁴ particles/cm³ (SD=5.6×10⁴ particles/cm³) whereas the background before the event was only 621 particles/cm³ (SD=113 particles/cm³). The maximum 1-second particle number concentration reached 1.9×10⁵ particles/cm³. Spearman Correlation factor between PM_{2.5} mass concentrations and particle number concentrations was 0.74 (p<0.01).

2AE.4

Spatiotemporal Estimates of Surface PM_{2.5} Concentrations in the Western U.S. Using NASA MODIS Aerosol Retrievals and Data Assimilation Techniques. S. MARCELA LORÍA-SALAZAR, Cesunica E. Ivey, Howard H. Chang, Jens Redemann, Heather Holmes, *University of Oklahoma*

Previous investigations have successfully estimated surface air pollution concentrations by creating statistical data fusion models in conjunction with aerosol satellite retrievals. However, the models developed for the eastern U.S. are often being used in the western U.S. without modifications. In this regard, these models are not robust in the western U.S. due to specific regional characteristics including: irregular topography that leads to complicated boundary layer physics; pollutant mixtures, heterogeneous vertical profiles of aerosol; and higher surface reflectance. With those considerations in mind, we apply a data fusion model to estimate surface PM_{2.5} concentrations in the western U.S. We also utilize new collections of aerosol products from the Terra and Aqua MODIS instruments as a spatial predictor of PM_{2.5} and emissions covariates from the NEI, which are prepared using the SMOKE emissions processing tool. The horizontal spatial resolution of the model is 12 km over the western U.S. and the temporal domain is daily over the study period of 2012-2013. The model incorporates spatially-resolved meteorological fields from WRF, elevation, population density, land cover information, surface reflectance, fire radiative power from MODIS, and plume injection height (PIH) from the Multi-Angle Implementation of Atmospheric Correction (MAIAC) as covariates to improve PM_{2.5} prediction performance. The novelty of this work relies on the use of high-resolution, temporally-resolved physics and emissions variables as covariates and satellite retrievals of PIH. Based on our previous research, the combination of high-resolution planetary boundary layer and PIH provides information on levels of aerosol pollution near-ground or aloft. Therefore, the covariates were selected to account for complex atmospheric physics and meteorological phenomena that govern the aerosol transport in mountainous regions. It is expected that by selecting a configuration of these physical variables, the PM_{2.5} concentration estimates in the data fusion model will be improved.

2AE.5

Evaluation of PM_{2.5} Exposures for an Environmental Justice Community Using a Low-Cost PM Sensor. Seung-Hyun Cho, Lisa Cicutto, Nalyn Siripanichgon, Michelle McCombs, Molly McCullough, Krysten Crews, Cindy Chang, Ryan Chartier, JONATHAN THORNBURG, Gregory Harshfield, Gregg Thomas, Michael Ogletree, Bradley Rink, *RTI International*

As low-cost air sensors become readily available, communities have opportunities to collect air quality and exposure data to improve their knowledge and contribute to environmental health research and policy decisions. Citizen scientists in Globeville, Elyria Swansea, an environmental justice community in Denver, with help of researchers, conducted air quality and personal exposure measurements for PM_{2.5} in the Summer and Fall of 2018 and the Winter of 2019. RTI MicroPEM sensors were placed at 12 sites as a neighborhood-scale sensor network, including three sites collocated with reference monitors. Nineteen participants measured their exposures by wearing MicroPEMs and completed time-activity diaries for three 72-hour monitoring periods over three seasons. Ambient PM_{2.5} data showed spatial variabilities with up to 3 times difference between site pairs. The highest PM levels were measured during the Summer, followed by Winter and Fall, with the difference between Summer and Fall reaching up to 2.5 times at one site. High temporal correlation ($r > 0.7$) with peaks at morning-evening commuting hours were observed at most sites, suggesting traffic pollution's influence on the community air quality. However, few sites such as parks showed PM increases in the mid-day during weekends. The individuals' personal exposure levels varied by day and season with real-time peak concentrations matching participant-reported exposure events related to lifestyle and activity types such as smoking and cleaning. On average, personal exposures were higher than the nearby ambient sensor measurement and lower than the near-road measurement. However, for the individuals with high exposure events, their personal levels were 6-24 times higher than nearby ambient sensor levels. Low-cost sensors have value in assessing the spatial and temporal variabilities of air quality and exposure at high resolution to support epidemiologic models. Additionally, the sensors are useful tools for behavioral intervention to reduce air pollution exposure. EPA Grant Number: RD83618701

2AE.6

Evaluation of the Size Distribution and Morphology of Submicrometer Particles Generated from Electrosurgical Tools. YUECHEN QIAO, Austin Andrews, Chase Christen, Brian MacLachlan, Samir Khariwala, Bernard Olson, Christopher Hogan Jr., *University of Minnesota*

Electrosurgical pencils (EPs) are widely used in a variety of medical procedures to aid in surgical cutting and cell and tissue coagulation. EPs are known to generate "surgical smoke", i.e. their use leads to the formation of a visible aerosol. The likely mechanism of aerosol formation is evaporation of organic material due to heating of tissue, followed by incomplete oxidation of this material in the gas phase, yielding particles. Therefore, the aerosol formation process may be similar to biomass burning and combustion processes, and may yield particles of similar size distribution and morphology to combustion systems. We examined the size distribution and morphology of particles produced by the operation of a monopolar EP applied to fresh bovine shoulder tissue at variable power settings. Measurements were carried out using (1) a differential mobility analyzer (DMA) and condensation particle counter (CPC) to determine mobility distribution functions in the 10 nm – 400 nm size range, (2) an aerodynamic particle sizer (APS) to determine aerodynamic particle size distributions in the 0.3 μm – 20 μm size range, (3) a DMA-electrostatic sampler to examine particle morphology at selected mobility equivalent sizes, and (4) a DMA- aerosol particle mass analyzer (APM) to determine the effective densities and mass-mobility scaling for particles. Collectively, measurements show a single mode, broad size distribution function of particles is produced in the 50 nm – 2 μm mobility diameter range, with a mode in the 100 nm – 200 nm range. Microscope analysis of particles revealed that spherical particles, fractal-like aggregates, and faceted, cubic particles can be produced simultaneously. Aggregate formation was confirmed through effective density determination. In total, results show that the particles produced during EP operation are morphologically extremely complex, suggesting there are multiple particle growth mechanisms occurring simultaneously, without sufficient time for internal mixing of the aerosol.

2AE.7

Changes in Emissions Rates and Exposure of PM_{2.5}, eBC, and UFP Attributable to the Renewal of a Bus Rapid Transit System Fleet. DANIELA MENDEZ, Sebastian Espitia, Andres Felipe Rosero, Boris Galvis, Ricardo Morales Betancourt, *Universidad de los Andes*

Transportation activities in urban centers are strongly associated with increased personal exposure to air pollutants. This situation can be exacerbated in developing economies due to older vehicle fleets and less stringent emission standards. In this work we focus on the Bus Rapid Transit System (BRT) of the city of Bogotá, in Colombia. This system is one of the largest in the world, with nearly 2.4 million trips daily. Previous work developed by the researchers has demonstrated that in-cabin concentration of PM_{2.5}, Black Carbon (BC), and ultra-fine particles (UFP) are alarmingly high inside the BRT buses and stations (Morales et. al., 2017; 2019). However, starting in July 2019, a new bus fleet will replace nearly 1400 18-year-old diesel-powered buses that are part of the current BRT system. The new fleet includes both EURO-VI natural-gas and EURO-V DPF-equipped diesel-powered buses. This fleet renewal is expected to significantly reduce emission rates of BC, PM_{2.5}, and UFP. We aim to characterize the evolution of BC, PM_{2.5}, and UFP fuel-based emission rates during the fleet renewal and to quantify the net change in exposure within the BRT system before and after the intervention. We selected seven points distributed throughout the BRT system to determine fuel-based emission factors by applying the carbon balance method. Carbon dioxide concentration was measured at 1 Hz with a NDIR sensor (LI-COR 830). UFP particles were measured using, both, an electric low-pressure impactor (Dekati, DMM-230) and a diffusion size classifier (DISCmini). Aethalometers and laser scattering devices were used to measure BC and PM_{2.5} respectively. Video recording was used to register all the events. Image analysis software was used to determine the timing of the passing of a BRT bus and its license plate. This information was compared to a data base of fuel type, mileage, and nominal emission standard. A total of 85 emission factors were calculated, obtaining an average of 2.01 mg PM_{2.5}/kg-fuel, 0.79 mg BC/kg-fuel and 1.49×10¹⁵ UFP/kg-fuel. Simultaneously, travelers in the system carrying portable measuring devices (micro-Aethalometers, DustTrack, and electrochemical cell CO sensors) performed natural trips in the system to determine the exposure concentrations. Our baseline phase results confirm the extreme exposure of the users of the current fleet, and highlights the large emission rates observed in these vehicles. It is expected to see a substantial positive change in the reduction of emissions and exposure with the implementation of the new fleet, and those measurements will be performed during the months of July and August.

2AE.8

Exposure to Inhalable Aerosols from Different Potential Factors in Building and Associated with Trace Elements. HYEON-JU OH, Jong-Ryeul Sohn, Jongbok Kim, *Rutgers, The State University of New Jersey*

Exposure to inhalable aerosols can be associated with health problems and, especially, the respirable fraction of particulate matter (PM) can penetrate the gas-exchange region of the lungs. Here we investigated three fractions of PM (PM_{2.5}, PM₄, PM₁₀) in indoors and outdoors, characterized of I/O ratios for PM under potential indoor (average occupancy) and outdoor factors (Asian dust, rain, wind, and snow days), and evaluated the fractions of trace elements in aerosols. Four places in the building were selected as sampling areas: a restaurant, a bank, a private school, and a general office. The concentrations and mass fractions (%) of 15 trace elements were determined using Inductively Coupled Plasma Mass Spectrometry. There was no significant difference of respirable aerosol (PM_{2.5} and PM₄) concentration in different indoor environments. PM₁₀ concentrations from outdoor factor were different only in windy day (at bank and private school) and snow day condition (at private school and office), while PM_{2.5} concentrations from outdoor factor were different in all investigated places. In all the events of outdoor factors except windy day, significant difference was observed in the restaurant and private school, which may be due to difference in ventilation efficiency. The ratios of trace elements in PM_{2.5} and PM₁₀ were different at various locations within the building. Although there was no difference in inhalable and respirable aerosol concentration at different locations within the building, the impact of outdoor factors is strongly supported by PM_{2.5}/PM₁₀ ratios of trace elements. This study shows that trace elements through the HVAC system affected the exposure to the indoor respirable aerosol, which could lead to adverse effect on the indoor air quality.

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2AE.9**Inhalation Exposure Characterization for Spray Products.**

KATHARINA SCHWARZ, Wolfgang Koch, *Fraunhofer ITEM, Germany*

Risk assessment regarding inhalation exposure for spray products requires information on aerosol emission in health related size ranges. Recently, there is an increasing demand in methods for exposure characterization, which consider the aerosol release under conditions of the actual application process including droplet maturation and shrinkage related to the evaporation of the solvents.

Therefore, a method based on the mass balance analysis of the matured aerosols in the respirable, thoracic and inhalable fraction under intended product use, relevant for the inhalation exposure of the spray user, has been developed. The exposure potential is quantified in terms of release fractions, defined as mass of aerosol generated in the three health-related size classes (respirable, res; thoracic, thor and inhalable, inh), normalized to total mass of liquid spray product released (release fractions, R_{res} , R_{thor} , R_{inh}). The three size fractions determined correspond to the three health-related size classes of airborne particles according to international standards (European standard EN 481 and ACGIH standard). These release fractions can be directly used as input parameters for exposure modelling using well-established models such as ConsExpo.

This method has been successfully applied for various spray products and applications, including biocidal droplet and foam spray applications, personal care products and spray processes in building protection. It provides reliable data on inhalation exposure potential for the different applications with release fractions covering several orders of magnitude. For droplet spraying processes, a simple, rough estimation could be derived for the thoracic release fraction based on well available properties of the formulation and the spraying technology.

In conclusion, the mass balance method takes into account the aerosol release potential under realistic conditions of use, i.e. the conditions relevant for the spray applicant. Thus, this new method contributes to the implementation of recommendations concerning the safety assessment of spray products.

2AE.10**Stability Testing of Large-Scale Whole-Body Inhalation Exposure Systems for Smoking Study.**

ZUOCHENG WANG, Amit Gupta, Steve Behringer, Zack Novak, Jan Satola, Ed Psurny, Sam Harbo, *Battelle*

E-cigarettes are less harmful than regular combustible cigarettes. However, more studies are necessary to investigate the long-term health effects from unexpected chemical changes, fugitive particles or fibres, and metals due to the varied combination of vehicle, flavor ingredients, nicotine, and device components. In this study, two large-scale whole-body inhalation exposure systems were set up and tested for stability (without animals) at high (1000 WTPM (wet total particulate matter) $\mu\text{g}/\text{L}$) and low (100 WTPM $\mu\text{g}/\text{L}$) concentrations from e-cigarettes and combustible cigarettes.

Two systems were set up, one for e-cigarettes and the other for combustible cigarettes. One whole-body Hazelton H-1000 chamber ($\sim 1 \text{ m}^3$, can hold 72 rats) was used for each exposure system. For e-cigarettes (button-activated), aerosol was generated by using linear smoking machines (Borgwaldt, LM24E) under CORESTA CRM81 puffing regimen (55/30/3). For combustible cigarettes (3R4F, University of Kentucky), cigarette smoke was generated by using rotary cigarette smoking machines (CH Technologies, JB2096) under Health Canada Intense Regimen (55/30/2). Each system was tested for 6 hours, run for stability at each concentration. Temporal stability and spatial uniformity were verified for each system. In addition, the following were quantified for e-cigarettes: tank weight loss, aerosol WTPM concentration, particle size distribution, nicotine, propylene glycol and glycerol concentrations; and the following were quantified for combustible cigarettes: butt length, aerosol WTPM concentration, particle size distribution, CO, nicotine, and aldehydes concentrations.

The results showed that the low and high target WTPM concentrations of 100 and 1000 $\mu\text{g}/\text{L}$ were achieved within the chamber for both systems. Aerosol particle size (mass mean aerodynamic diameter) ranged from 0.9 to 1.0 μm for e-cigarette and from 0.7 to 0.9 μm for combustible. Chamber stability and uniformity were within specifications (<10%) for all the tests.

2AE.11**Indoor and Outdoor PM₄ Continuous Monitoring in a Low Income Community of Highveld Priority Area of South Africa.**

Joseph Adesina, Stuart Piketh, Marvin Qhekwana, Roelof Burger, Brigitte Language, Gabi Mkhathswa, *North-West University, South Africa*

This study was carried out in a low income community situated in the proximity of three coal-fired plants to better understand the relationship between indoor and ambient respirable particulate matter (PM₄). The findings were to serve as a guide in the implementation of air quality offset guidelines seeking to address environmental air pollution due to residential solid fuel combustion. Two formal Reconstruction and Development Programme (RDP) houses were selected for the study with a further classification of solid fuel burning and non-solid fuel burning. Continuous monitoring were carried out in both houses during summer and winter seasons. At solid fuel burning house the winter average concentration ranges between 60.9 μgm^{-3} and 208 μgm^{-3} while at non-solid fuel burning it ranges between 15.3 μgm^{-3} and 84.2 μgm^{-3} . In both houses the national ambient air quality standard (NAAQS) of PM_{2.5} (40 μgm^{-3}) was exceeded during the winter season. The summer had a cleaner indoor concentration where the 24-hr average concentration hardly exceeded the required national standard. The concentration ranges between 17.4 μgm^{-3} and 36.6 μgm^{-3} at the solid fuel burning and between 14.2 μgm^{-3} and 39.9 μgm^{-3} at the non-solid fuel burning. During mornings and evenings, the indoor concentration were higher than the outdoor in both houses, these coincides with the burning pattern in this community but in the afternoon the outdoor sometimes were higher than the indoor perhaps as a result of the pollution from the power plants in the neighborhood of the township. There were no significant correlations between indoor and outdoor concentration during the winter, but the correlations were good for both houses during the summer.

2AE.12**Organic Extracts of PM_{2.5} in Seoul Mediates Neutrophilic Inflammation and Aging in Lung Epithelial Cells.**

JIEUN PARK, Kyoung-Hee Lee, Jongbae Heo, Chang-Hoon Lee, Seung-Muk Yi, Chul-Gyu Yoo, *Seoul National University, Seoul, Korea*

Ambient fine particulate matter with an aerodynamic diameter of 2.5 μm or less (PM_{2.5}) is well known to be associated with adverse health effects. Several studies have been providing evidence that PM_{2.5} leads to inflammatory response by provoking oxidative stress. Airway epithelial cells are the first line of defense against the inhaled PM_{2.5} and key effector cells in the pathogenesis of several lung diseases. The objective of this study was to assess the effect of non-polar organic compounds of PM_{2.5} (high concentration events in Seoul) in lung epithelial cells.

PM_{2.5} samples were collected for 24-hr in Seoul, South Korea. Selected twelve samples for the PM_{2.5} events included four seasons and punched filters (4cm x 4cm) were extracted to be used for non-polar organic compound analysis and *in vitro* experiments. Organic compounds were analyzed using a GC-MS.

The organic extracts of PM_{2.5} samples were exposed to BEAS-2B. The results showed that the extracts specifically induced IL-8 production, but not IL-1 β , IL-6, TNF- α , and IL-17. The PM_{2.5} samples activated extracellular signal-regulated kinase (ERK) and pretreatment of ERK inhibitor (U0126) completely suppressed PM_{2.5}-induced release of IL-8, which suggest that PM_{2.5}-induced IL-8 production is dependent on ERK activation. Aging in lung epithelial cells impairs lung function. We found that PM_{2.5} significantly increased the expression of aging markers such as p21 and p27. ERK activation, IL-8 production, and up-regulation of aging markers were also observed in primary human airway epithelial cells. These results positively correlated with the level of PAHs and n-Alkanes in PM_{2.5}.

Our findings suggest that non-polar organic compounds of PM_{2.5} mediate neutrophilic inflammation and aging and chemical composition of organic compounds might be important to determine the toxicity of PM_{2.5} in respiratory system.

2BC.1

Effects of Fuel Moisture Content on Biomass Emissions from a Rocket-Elbow Cookstove. Lizette Van Zyl, Jessica Tryner, Kelsey Bilsback, Nicholas Good, Arsineh Hecobian, Amy P. Sullivan, Yong Zhou, Jennifer Peel, JOHN VOLCKENS, *Colorado State University*

Exposure to air pollution from solid-fuel cookstoves is a leading risk factor for premature death; however, the effect of fuel moisture content on air pollutant emissions from solid-fuel cookstoves remains poorly constrained. The objective of this work was to characterize emissions from a rocket-elbow cookstove burning wood at three different moisture levels (5%, 15%, and 25% on a dry mass basis). Emissions of carbon dioxide (CO₂), carbon monoxide (CO), methane, fine particulate matter (PM_{2.5}), PM_{2.5} elemental carbon (EC), PM_{2.5} organic carbon, formaldehyde, acetaldehyde, benzene, toluene, ethylbenzene, and xylenes were measured. Emission factors (EFs; g·MJdelivered⁻¹) for all pollutants, except CO₂ and EC, increased with increasing fuel moisture content: CO EFs increased by 84%, PM_{2.5} EFs increased by 149%, formaldehyde EFs increased by 216%, and benzene EFs increased by 82%. Both modified combustion efficiency and the temperature at the combustion chamber exit decreased with increasing fuel moisture, suggesting that the energy required to vaporize water in the fuel led to lower temperatures in the combustion chamber and lower gas-phase oxidation rates. These results illustrate that changes in fuel equilibrium moisture content could cause EFs for pollutants such as PM_{2.5} to vary by a factor of two or more across different geographic regions.

2BC.2

Increasing Global Lung-Cancer Risk Due to Biomass Combustion in the 21st Century. Sijia Lou, MANISHKUMAR SHRIVASTAVA, Richard Easter, Jerome Fast, Philip Rasch, Huizhong Shen, Staci L. Simonich, Shu Tao, Alla Zelenyuk, Steven Smith, *Pacific Northwest National Laboratory*

This study will present results of global atmospheric model simulations investigating how biomass combustion will increase lung-cancer risk in the 21st century. Simulations account for measurements that have shown how organic aerosol coatings shield cancer causing polycyclic aromatic hydrocarbons (PAHs) from atmospheric chemical degradation. Global emissions of toxic polycyclic aromatic hydrocarbons (PAHs) that are emitted from combustion of biofuels and fossil fuels are expected to change significantly in the future due to shifts in land-use, regulatory policy, and technology changes. Representative concentration pathways are used to explore plausible future emissions and climate-change scenarios, and identify how lung-cancer risk due to PAH exposure could change in the future relative to 2008. Globally, residential biofuel is found to be the largest contributor to PAH emissions in both 2008 and 2050. Benzo(a)pyrene, one of the most carcinogenic PAHs is used as an indicator of PAH-associated lung cancer risk. Model simulations indicate that the global PAH-associated lung-cancer risk is projected to exceed WHO acceptable limit guidelines even in 2050. In developing regions of Africa and South Asia, the increased agricultural waste burning and shifts to traditional biomass-use for energy lead to an increase in lung cancer risk by up to 60% in 2050. However, our study also indicates that the “climate benefit” for BaP can partially offset the emission change-associated increment of lung cancer risk in these developing regions.

2BC.3

The Impact of Biomass Fuel Emissions on Women's Health in Rural Punjab. NABEELA FARAH, *University of Agriculture, Department of Rural Sociology*

Indoor air pollution due to the burning of biomass fuel in developing countries is a well-established health hazard. In rural Punjab, biomass fuel is used as a primary source for cooking and heating. Biomass burning contains hundreds of compounds that have serious impact on women's health. This study estimated the health effects of exposure to smoke from burning of agricultural waste, dung cakes and wood used in three districts of Punjab. Daily biomass fuel exposure and health outcomes were self-reported. Data included a survey of 480 women and interactions of fuel, stove and kitchen use were conducted to evaluate the health effects. These data were analyzed by using ordinal and multivariate logistic regression models and presented in the form of mediation, moderation and interaction effects. The results show the odds of having more frequent headaches increased (OR =3.62, $p=.001$) when dung cake was used in conjunction with blocked kitchen. Similarly, the odds of having more frequent chest pain increased (OR =8.05, $p=.026$) when wood was used in a mid-brick stove. The interaction between dung cake and time spent in the kitchen was significant. It results in higher odds of having more frequent cardiac disease by a factor of 5, when dung cake was used for 7-9 hours in the kitchen. Incomplete combustion caused by insufficient amount of air accounts for a strong association between wood use and coughing. Findings show the relationship between income and breathing problem was partially mediating by the use of agricultural waste and the odds of more frequent breathing problems in the low income group were more than double (OR=2.32, $p=.002$) that of the high income group. This study did not find the interaction of kitchen ventilation or kitchen construction with women's health.

2BC.4

Quantifying the Impact of Biomass Burning on Aerosol Concentrations in Bogota, Colombia: Detection of Biomass Burning Tracers and Model Simulations. Maria Alejandra Rincón, Amy P. Sullivan, Juan Manuel Rincón, Juan Felipe Mendez, Karen Ballesteros, RICARDO MORALES BETANCOURT, *Universidad de los Andes*

Biomass burning (BB) aerosol particles significantly deteriorate air quality in many regions around the world and impact climate through both direct and indirect aerosol effects. Recent studies suggest that a significant portion of the seasonal variations in PM pollution levels in the city of Bogota, Colombia, can be explained by regional transport of BB plumes from agricultural burns and wildfires. This contribution seems to be more important during the dry months (January-April) compared to the wet season (July-September). In this work we aim to quantify the local and regional contributions of BB aerosols to PM concentrations in the city by detecting biomass burning tracers in $PM_{2.5}$ samples collected in Bogota. Chemical transport modelling with WRF-Chem and back trajectory analysis are also performed to further apportion the local versus regional contributions. We conducted two field campaigns during 2018 simultaneously at two sites in the city of Bogota, one during the dry season and the other during the rainy season. Over 120 $PM_{2.5}$ 24-hour samples were collected in quartz filters. Chemical composition of the samples was carried out to determine carbonaceous fraction (OC, EC), water soluble organic carbon (WSOC), smoke tracers including levoglucosan, as well as other water soluble organic species. In addition, inorganic ions and some metals were determined. To interpret the results, MODIS active fire data was used to select those fires with the potential to impact local air quality. Time series of selected fires were analyzed with concentrations of BB tracers within different buffer from Bogota. Mean daily $PM_{2.5}$ concentration during the dry season was $20 \mu\text{g}/\text{m}^3$ and $7.5 \mu\text{g}/\text{m}^3$ during the rainy season. OC was the dominant component of $PM_{2.5}$ in both field campaigns with a larger contribution during the rainy season. A large WSOC/OC ratio of 0.63 was observed in the dry season samples. We found a persistent presence of BB tracers in the samples for both field campaigns with higher concentrations of Levoglucosan during the dry season. A stronger association between BB tracers was observed in the dry season compared to the rainy season samples. Regional chemical transport model simulations with WRF-Chem including fire emissions further confirm the seasonal impact of BB to PM during the dry season. This study is the first to report full chemical composition analysis of $PM_{2.5}$ in the city, highlighting the prevalence of organic aerosols and the large fraction of WSOC. Our results suggest that secondary organic aerosols are significant in this urban environment.

2BC.5

Measurements to Determine Mixing State of Black Carbon Emitted from the 2017/2018 California Wildfires and Urban Los Angeles. JOSEPH KO, Trevor Krasowsky, George Ban-Weiss, *University of Southern California*

The importance of atmospheric black carbon (BC) and its effects on climate have been established, but uncertainties remain regarding its impacts at different spatiotemporal scales. Here, we seek to understand the mixing state evolution of BC emitted from various sources and aged over different timescales, using measurements in the Los Angeles (LA) region. We measured refractory black carbon (rBC) with a single-particle soot photometer (SP2) on Catalina Island, California. During the first campaign (September 2017), the sampling location was upwind of the dominant regional sources of BC (i.e., urban emissions from the LA basin). In the second and third campaigns (December 2017, November 2018), atypical winds advected rBC to our sampling location from California wildfires and urban emission. We observed the largest number fraction of thickly coated particles (f_{BC}) and coating thickness (CT_{BC}) during the first campaign (~ 0.27 and ~ 36 nm, respectively), and during a period of the third campaign when we suspect that measured rBC was dominated by long-range transport from the Camp Fire in Northern California (~ 0.35 and ~ 52 nm, respectively). In contrast, during periods when measured rBC was dominated by particles from Southern California fires or urban emissions, we found lower f_{BC} and CT_{BC} values (~ 0.03 and ~ 0 -10 nm, respectively). We conclude that an aging timescale on the order of \sim hours is not long enough for rBC to become coated thickly in the LA region. We found that measured rBC acquired substantial coatings when aging timescales were greater than ~ 24 hours. Results presented here suggest that rBC mixing state is highly dependent on emissions source-type and atmospheric context since the CT_{BC} (per hour of atmospheric aging) was found to be smaller than what has been previously reported in literature in other locations around the world.

2BC.6

Prediction of Organic Aerosol Precursor Emission from Wood Pyrolysis. MARIAM FAWAZ, Tami Bond, *University of Illinois at Urbana Champaign*

Emission of organic aerosols (OA) from wood combustion is responsible for a large percentage of primary organic aerosols in the atmosphere, most of which are released during the pre-ignition phase when pyrolysis is occurring. In this work, we present a pyrolysis model that predicts the release of the class of gases that includes OA precursors, called heavy gases. Temperature and mass loss in modeled pyrolysis are validated against experimental data from a controlled isothermal cylindrical reactor that gives highly reproducible pyrolysis, with instantaneous mass loss rates within 10% between replicate experiments.

We demonstrate the potential of using pyrolysis modeling in understanding the emission of OA from wood combustion. Heavy gases are the products of tar secondary reactions, where tar is formed as a condensed phase from primary pyrolysis reactions. We use the model to calculate the yield of emission and release rate of heavy gases. Maple wood of dimensions 14x3.8x2.9 cm was used at three reactor temperatures (400C, 500C, and 600C). The yield of heavy gases increased from 70% to 80% by mass when the pyrolysis temperature changed from 400C to 600C. The rate of emission of heavy gases showed one broad peak at 400C and two sharp peaks at 600C throughout pyrolysis. The magnitude of peak emission rate was higher at 600C than 400C. We attribute the multiple peaks in emission rate to the large thermal gradient that forms initially between the surface and center at high temperature. During pre-ignition, higher heat flux promotes the rapid release of heavy gases and the subsequent release of high OA during this important initial period of wood heating that precedes combustion.

2BC.10**Observations of Strong Secondary Aerosol and Ozone Formation in Biomass Burning Plumes in Southern Africa.**

VILLE VAKKARI, Johan Paul Beukes, Miroslav Josipovic, Pieter G. van Zyl, *Finnish Meteorological Institute, Helsinki, Finland*

Biomass burning (BB) is a major source of aerosol particles and trace gases globally with significant implications for air quality and climate. Particulate matter (PM) emissions and ozone (O₃) formation during plume transport can degrade air quality hundreds of kilometers away from the fire. Simultaneously, the large variability in BB emissions exerts significant uncertainty in climate predictions. Globally, one of the largest sources of BB aerosols is southern Africa, where savanna and grassland fires are frequent during the dry season from June to October. Here, we utilize continuous measurements of submicron aerosol size distribution, black carbon (BC) and trace gases at Welgegund, South Africa (26.57S, 26.94E) from May 2010 to January 2016. During this period we identified 130 smoke episodes totalling >400h of in-plume measurements. We observed strong secondary aerosol formation in smoldering daytime plumes with >3x PM enhancement in less than 4h of ageing. Also O₃ formation was substantial during daytime ageing, with excess O₃ to excess CO ratio reaching 0.25 for >3h old smoldering plumes. In flaming cases no net PM increase occurred, resulting in an average increase in PM by a factor of 2. This suggests that a major fraction of the discrepancy between top-down and bottom-up BB emission estimates may be due to missing near-fire secondary aerosol formation. Furthermore, secondary aerosol formation during ageing affects strongly the submicron size distribution: during the first 3h we observed modal mean diameter grow from 70nm to 120nm.

2BC.11**Seasonality and Inter-site Variability in Cookstove Emissions Measured in a Multi-year 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*

Particulate and gaseous pollutants emitted from biomass stoves have adverse health and climatic impacts. This study characterizes cookstove emissions measured during a multi-year intervention study in two rural areas (Kullu in Himachal Pradesh; Koppal in Karnataka) in India. 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-home emission measurements were conducted before and after introduction of the new stove, and include real-time concentrations of carbon dioxide, carbon monoxide (CO), particle light scattering and absorption, and gravimetric PM_{2.5} and organic/elemental carbon analyses. The study had three ~3-month-long measurement periods (baseline: BL, follow-up-1: F1, follow-up-2: F2) in each location. We observed inter-period and inter-site variability in traditional stove emissions. For example, mean PM_{2.5} emission factor (EF) of traditional stove in Koppal was 51% and 32% higher in F2 than BL and F1 respectively. In Kullu, PM_{2.5} EF was significantly lower in F1 relative to BL (40%) and F2 (32%). Multilinear regression models were used to evaluate sources of emission variability including season, location, fuel properties (e.g. moisture content: MC and fuel use), relative humidity (RH) and cooking duration. Models including MC, RH, CO EF and single scattering albedo (SSA) as predictors explained 58% and 52% variability in PM_{2.5} and OC EF respectively. Season, fuel use, MC, OC and EC EF explained ~75% variability in SSA. LPG stoves had the lowest pollutant EFs of all the stoves in this study. Mean PM_{2.5} (1.8 ± 2.4 g kg⁻¹) and CO EF (34.3 ± 23.1 g kg⁻¹) of LPG were 3 and 2 times lower respectively than all biomass stoves. However, in-home mean PM_{2.5} and CO EFs were ~36 and 2 times higher respectively than values measured during lab testing. Our analysis indicates sources other than fuel (e.g. food) contributed to high emission in some LPG tests.

2BC.12

Identifying Functional Groups and Predicting OC-EC in Cookstove Source Emissions. EMILY LI, Michael Hays, James Jetter, Guofeng Shen, Satoshi Takahama, Ann Dillner, *U.S. EPA*

Globally, billions of people burn fuels indoors for cooking and heating, which contributes to millions of premature deaths and chronic illnesses annually. Additionally, residential burning contributes significantly to black carbon emissions, which are estimated to have the highest global warming impact second to carbon dioxide. In this study, we use Fourier transform infrared spectroscopy (FTIR) to analyze PM_{2.5} emissions collected on Teflon membrane filters from fifteen cookstove types and five fuel types. Emissions from three fuel types (charcoal, kerosene, and red oak wood) were above the minimum detection limit for functional group analysis. We present distinct spectra for these three fuel types. We also show that FTIR spectra can be used in multivariate linear regression analysis in a data-driven machine learning model to predict organic carbon and elemental carbon (OC/EC) ratios, which are traditionally measured using destructive, time-consuming thermogravimetric methods. Since FTIR measurement is non-destructive and only takes three minutes per sample, this ability to predict OC/EC from FTIR spectra can potentially significantly reduce the need for thermogravimetric OC/EC measurements.

2BC.13

Black Carbon Emissions from Residential Wood Combustion and Drivers for Further Research. REBECCA TROJANOWSKI, Arthur J. Sedlacek, Ernie R. Lewis, Vasilis Fthenakis, Thomas Butcher, *Brookhaven National Laboratory*

Particulate matter (PM) from residential wood combustion (RWC), for both heating purposes and cooking, contains both organic (carbon containing) and inorganic (salts and sulfates) components. These particles impact air quality in terms of health effects and visibility as well as the climate. The climate may be affected indirectly by cloud formation or directly in terms of scattering or absorbing light. Particles that scatter solar radiation increase Earth's albedo and have a negative climate forcing impact. However, some particles absorb radiation and have a positive climate forcing impact by converting the absorbed energy into heat. Black carbon (BC) and some organic matter (OM) aerosols are known to have this affect.

While advancements in technology such as catalytic wood stoves and boilers, secondary combustion chambers, and automatic fuel-fed appliances (pellets and woodchips) have led to the reduction of total PM, very few studies have studied the BC emissions from these technologies and the overall effect of switching from traditional wood heating appliances to fewer polluting technologies. To better understand the sources of BC, more current information and better emission inventories are needed. Policy-relevant research needs improved BC emission inventories on sources and their operating conditions, and BC mitigation to promote advanced combustion technologies. Characterizing BC from sources will also help reduce model uncertainty and improve predictive power of climate models. Brookhaven National Laboratory (BNL) has begun to quantify the BC associated with controlled residential biomass combustion by utilizing laser-induced incandescence; specifically using the single-particle soot photometer (SP2). Columbia University will then work with the data to help update emission inventories and model predictive power.

2BC.14

Measuring Particle Number Concentration from Woodburning Stoves. NICOLE VITILLO, Patricia Fritz, Jake Lindberg, Thomas Wainman, Nathan Walz, Todd Crawford, Rebecca Trojanowski, Thomas Butcher, *New York State Dept. of Health*

The 2018 Wood Stove Design Challenge (WSDC) was held in November on the National Mall, in Washington D.C. During this event, three wood burning stoves were tested to determine their emissions characteristics according to a protocol developed specifically for the event. The testing protocol was developed to challenge the stoves to perform well under loading conditions that are more representative of real-world use.

As part of the WSDC, our team measured the Particle Number Concentration (PNC) in representative flue gas samples using the TSI NanoParticle Emissions Tester 3795 (NPET). The NPET is a portable instrument with internal dilution and built-in catalyst for removal of volatiles. It uses condensation particle counter technologies to measure sub micron particles at concentrations below 5,000,000 particles /cm³. The NPET is currently used for in-use emissions and compliance testing of diesel-powered machinery with diesel particulate filters in accordance with the Swiss Regulation SR 941.242, which defines regulatory particle number concentration (PNC) limits.

In this work, we describe incorporating the NPET device in a non-regulatory sampling capacity along with other biomass sampling instruments, show the results of PNC measurements made during the sampling campaign, and discuss the trends in PNC emission which arise during different phases of the operational protocol. During the WSDC, our team also made measurements of the flue gas composition and the emission of Black Carbon (BC) species, which will be discussed separately.

2BC.15

In-Stack Aethalometry Measurements of Woodburning Stoves. JAKE LINDBERG, Patricia Fritz, Nicole Vitillo, Rebecca Trojanowski, Thomas Butcher, Thomas Wainman, Nathan Walz, Todd Crawford, *New York State Dept. of Health*

The 2018 Wood Stove Design Challenge (WSDC) was held in November on the National Mall, in Washington D.C. During this event, three wood burning stoves were tested to determine their emissions characteristics according to a protocol developed specifically for the event. The testing protocol was developed to challenge the stoves to perform well under loading conditions that are more representative of real world use.

As part of the WSDC our team measured the emission of black carbon (BC) species using two instruments; the Brechtel Tri-color Absorption Photometer Model 2901(TAP) and the Thermoscientific Personal DataRAM pDR-1500 (pDR). The TAP measures light absorbance at three wavelengths 365, 528, and 652 nm. Using the red light absorption measurements we estimated the real time BC concentration in the flue gas using standard practices. We also used the pDR, which measures light scattering at the 880 nm wavelength, to produce a separate estimate of BC concentration. Additionally, in order to better characterize the flue gas aerosol we used the differences in the absorption of 370 and 880 nm wavelength light reported by the TAP to calculate an effective Angstrom-Absorption Exponent (AAE).

In this work we report: the BC measurements from the sampling campaign, discuss the trends in BC emission during different phases of the operational protocol, and show how aethalometric measurements of flue gas can be a useful tool, to help understand the operation of combustion appliances through changes in carbon characteristics. During the WSDC our team also made measurements of the flue gas composition and the Particle Number Concentration (PNC), which will be discussed separately.

2BC.16**Source Apportionment and Mass Measurement of Fine Particulate Matter Arising from Massive Southern Oregon and Northern California Fires during the Summer of 2018.**

DAVID GOBELI, Jennifer Brown, George Allen, *Met One Instruments, Incorporated*

Black carbon "BC", brown carbon "BrC", and continuous gravimetric PM_{2.5} were measured in Grants Pass Oregon during a series of devastating, lightning induced wildfires in southern Oregon and northern California during the summer and fall of 2018. The equipment was set up at a monitoring site which at times was within a few miles of one or more of the active fires. BC and BrC were measured using portable and rack-mounted, tape-based carbon monitors of two and ten illumination wavelengths respectively. Total mass in the form of PM_{2.5} was continuously measured during the event using a class 3 US-EPA designated beta attenuation mass monitor "BAM" and a high-temporal resolution optical PM monitor. All monitors were collocated. Monitoring results reveal very good correlation between BrC and PM_{2.5} and fair to good correlation between BC and PM_{2.5}. BC, measured at 950 nm was typically 2-5% of gravimetric PM_{2.5}. BC, which is normally present in low concentrations (< 0.300 µg/m³) because of the low population density of the region was measured at concentrations approaching 10 µg/m³ during the event. BrC, which is normally almost non-existent in the region during the summer months, except in cases of forest fires, was recorded at concentrations close to 50 µg/m³ using UV (370 nm) illumination only. Sandradewi's and other methods for source apportionment were also evaluated using different combinations of illumination wavelengths, and equivalent black carbon "EBC" wavelengths. Wide variations in the BrC/EBC fractions were observed at the commonly used 470 nm/950 nm illumination combination over time, perhaps because of varying distances between active fire events and the fixed monitoring sites. In addition, wide variations were noted in the differences between reported BrC/EBC fraction as a function of UV and IR illumination wavelength combinations.

2BC.17**Smoke Aerosol Radiocarbon Measurements from Indonesian Fires Provide Evidence for Burning of Millennia-aged Peat.**

ELIZABETH WIGGINS, Claudia Czimczik, Guaciara dos Santos, Xiaomei Xu, Yang Chen, Jim Randerson, Charles Harvey, Fuu Ming Kai, Liya Yu, *NASA*

During the boreal fall of 2015, El Niño induced drought severely exacerbated fires in Indonesia. The fires released an enormous amount of fine particulate matter and created an immense regional smoke cloud that severely degraded air quality for millions of people across Southeast Asia. Although previous studies suggest peat burning was the main contributor to emissions in this region, drought caused by El Niño can also increase agricultural waste burning in plantations and deforestation fires. Significant uncertainty remains with respect to partitioning fire emissions across different landscape sources. In this study, we measured the total carbon concentration and radiocarbon content ($\Delta^{14}\text{C}$) of carbonaceous aerosols collected in Singapore, a major city downwind of the fire emissions, to determine the dominant source of these haze-inducing aerosol emissions. The $\Delta^{14}\text{C}$ of fire derived aerosol was $-76 \pm 51\%$, corresponding to a carbon pool of combusted organic matter with a mean turnover time of 800 ± 420 yr. Our observations indicated that smoke plumes reaching Singapore originated predominantly from the burning of peat (~85%), and not from agricultural waste burning or deforestation fires. The mean age of the carbonaceous aerosol, which predates the Industrial Revolution, highlights the importance of improving peatland fire management during future El Niño events for meeting climate mitigation and air quality commitments.

2BC.19

Networks of Multi-wavelength MicroAeth Monitors Provide Tracer of Ground Level Air Pollution Impacts of Long Range Transport of Wildfire Plumes in NYC. STEVEN CHILLRUD, Qiang Yang, Beizhan Yan, Mark Arend, Fred Moshary, Jeff Blair, Yonghua Wu, Tanja Dobovicnik, Michele Markowitz, Wade McGillis, *LDEO of Columbia University*

The frequency and intensity of wildfires is increasing, in part due to climate change. The plumes from larger wildfires can be tracked via remote sensing for thousands of miles but whether they lead to increased exposure to humans or wildlife depends upon whether and when the plume is mixed down to ground level. Routine air pollution monitoring data can show temporal increases for a wide variety of air pollutants (e.g., PM_{2.5}, carbon monoxide, Ozone, etc.) that are also impacted by other sources, making assessments reliant upon having long term data sets and having other key data (meteorological, LIDAR and ceilometer data). Here we focus on wildfire transport events that reached ground level of NYC based on remote sensing, NOAA back trajectories and local ceilometer and lidar data and compare their impact on a more specific tracer of wildfire plumes- multiwavelength microAeth (MA350s, Aethlabs) data collected at two locations- one in the highlands of Northern Manhattan and the second that captures the upwind air mass roughly 15 miles north of the other site. Additional data not already mentioned above are also available for these events, including: NOAA products for backward trajectories and HRRH column smoke for the wild fire plumes showing it reaching NYC and NYS, and data collected from microAeths in the San Francisco area confirm the ultraviolet (UV) signature of the wildfire event. The multi-wavelength microAeth data clearly shows a strong wildfire signal based on the strong UV signature of wildfire emissions whose strength is well timed with the LIDAR and Ceilometer data and of equal magnitude at the two sites described above consistent with an upwind source far away; in comparison due to local emissions, the black carbon data at the urban site is much higher than that at the upwind site.

2BC.20

Impact of Long-Range Transport of Central America Biomass Burning Emissions on Air Quality in Texas. QIANJIN ZHENG, David Ramirez, Min Zhong, *Texas A&M University-Kingsville*

Every spring, transported smoke from Central America reaches South Texas resulting in elevation of daily PM_{2.5} and impaired air quality. The objectives of this study are to examine the transport of smoke, analyze the spatial distribution of air pollutants, and quantify the impact of biomass burning on local air quality using the Weather Research and Forecasting model coupled with Chemistry model (WRF-Chem). The model domain covers Central America, Mexico, and the southern U.S. at 18 km horizontal resolution. Four gas-phase and aerosol mechanisms were tested to select the best mechanism in predicting gases, aerosols, and aerosol direct and indirect effects. Then we employed two global fire emission inventories, the Fire INventory from NCAR (FINN) and the Global Fire Emissions Database (GFED), for the air quality simulations. Overall, the model reproduced the spatial and temporal patterns of PM_{2.5} which were consistent with the observed data. CBMZ-MADE/SORGAM mechanism provided the best simulation results which were closer to observations with a correlation coefficient of 0.676, among the four tested mechanisms. Smoke plumes from Central America spread across certain areas in South Texas and affected the local air quality, with enhancements of up to 15 ppb O₃ and 20-30 µg/m³ of PM_{2.5}. Moreover, it took around two days to lower down the PM_{2.5} concentrations to the background level. Our work indicated that the boundary conditions from the WRF-Chem model form both gas-phase and aerosol pollutants contributed significantly in the simulation of all four mechanisms. Our study highlighted that long-range transport of biomass burning emissions should be considered when evaluating the relative effectiveness of local emission control programs, which could be helpful on the determination of compliance with National Ambient Air Quality Standards.

Keywords: Biomass Burning, WRF-Chem, Central American, Texas, Air pollution, Air quality

2BC.21**Single Particle Mass Spectrometry Observations of Long Range Transported Biomass Burning Aerosols in Michigan.**

JAMY LEE, Brady Anderson, Peter-Philip Booth, Jun Liu, Peng Xian, Kerri Pratt, *University of Michigan*

Wildfires are a major source of biomass burning particles released into the atmosphere. Biomass burning particles directly impact climate and cause adverse health effects. In recent years, the area burned in the western United States from forest fires has increased. Biomass burning particles released from these fires can travel long distances and impact air quality far downwind. During September 2018, aerosol time-of-flight mass spectrometry (ATOFMS) was used to measure the size and chemical composition of individual atmospheric particles in real-time in Ann Arbor, Michigan. We utilized the Navy Aerosol Analysis and Prediction System (NAAPS) reanalysis and the NOAA Hazard Mapping System Fire and Smoke Product (HMS) to identify smoke traveling from multiple fires across North America to Michigan. A significant portion of the days when smoke was prominently detected was characterized by biomass burning particles coated with oxidized organic carbon, ammonium, nitrate, and sulfate, yielding insights into the long-range aging of wildfire smoke particles.

2BC.22**Emission and Evolution of Submicron Aerosol Composition in Wildfire Smoke in the Western United States.**

LAUREN GAROFALO, Ezra Levin, Matson A. Pothier, Sonia Kreidenweis, Delphine K. Farmer, *Colorado State University*

The number and intensity of wildfires in the western United States is increasing, and the relative impact of emissions from wildfire on regional and global atmospheric composition is becoming more significant. However, aerosol emissions from wildfire are poorly understood and difficult to quantify due to variability in environmental and fire conditions that impact particle emissions. Measurements of particles from wildfire inherently occur downwind of the fire, and can be influenced by chemistry and dilution effects in the near field where smoke is less than 2 hours old. This dilution and chemistry continues as a wildfire plume evolves and is transported. Here, we investigate the emissions, evolution, and chemistry of aerosol from wildfires in the near field with data from the Western Wildfire Experiment for Cloud Chemistry, Aerosol Absorption, and Nitrogen (WE-CAN). We describe the chemical composition of submicron, non-refractory aerosols in the dynamic environment of wildfire smoke plumes as measured by high-resolution time-of-flight aerosol mass spectrometry (HR-TOF-AMS; Aerodyne, Inc). We also discuss black carbon (BC) as measured by single particle soot photometry (SP2; Droplet Measurement Technologies). Organic aerosol (OA), inorganic aerosol, and BC emissions vary due to fuels and fire conditions, which can differ not only across different fires, but also within a single wildfire. These primary emissions evolve as the plume is simultaneously diluted by background air leading to dilution-driven evaporation and photochemical aging. Specifically, we will discuss the emission and evolution of inorganic species (NH_4^+ , SO_4^{2-} , Cl^- , NO_3^-) in submicron aerosol in wildfire smoke plumes. Characterizing aerosol emissions from wildfires and how chemical oxidation and physical dilution compete in the smoke plume is crucial to understanding the effects of particle emissions from wildfire on air quality and climate.

2BC.23**Characterization of Biomass Burning Aerosols Produced in the Laboratory with a Light-Scattering Aerosol Mass Spectrometer and Ultraviolet/Visible Absorption Spectroscopy of Water-Soluble Organic Carbon.**

ANN M. MIDDLEBROOK, Rebecca Washenfelder, Alessandro Franchin, Gabriela Adler, Matthew Coggon, Kara D. Lamb, Katherine M. Manfred, Joshua P. Schwarz, Vanessa Selimovic, Nick Wagner, Caroline Womack, Robert J. Yokelson, *NOAA ESRL*

During the 2016 NOAA FIREX project at the Missoula Fire Sciences Laboratory, fires of known fuel type and properties were ignited to characterize their direct emissions with a large variety of new sampling methods. During these experiments, we measured the non-refractory components of the smoke particles using an Aerodyne compact time-of-flight aerosol mass spectrometer (AMS) with a light scattering module. One type of experiment involved sampling when the exhaust vent was closed to fill the room with smoke for several hours (so-called "room burns"), that allowed us to perform several kinds of studies related to the volatility, photochemical aging, and further characterization of the aerosols. The unique measurements obtained with the light-scattering module provide some insight on how the total mass of biomass burning organic aerosol is detected with an AMS. In addition, we investigated potential relationships between the non-refractory, submicron AMS chemical composition and the wavelength-dependent absorption of aerosol water-soluble organic carbon for various experimental conditions. These findings will be compared with preliminary results from the 2019 FIREX-AQ field study aboard the NOAA Twin Otter aircraft.

2BC.24**Characterizing Aerosol Emissions from Wildfires in the Western US.**

EZRA LEVIN, Kevin Barry, Kathryn Moore, John Ortega, Lauren Garofalo, Matson A. Pothier, Darin Toohey, Mike Reeves, Jakob Lindaas, Ethan Emerson, Delphine K. Farmer, Sonia Kreidenweis, Paul DeMott, Emily Fischer, *Colorado State University*

Wildfires are a major source of fine and accumulation mode aerosol in the western United States, especially during the summer months. Increased fire activity has been observed in recent years and wildfires are predicted to become even larger and more numerous under future climate scenarios. Emissions from wildfires increase aerosol number and mass concentrations locally and can also be transported over long distances, leading to regionally elevated aerosol loadings. Because of their high concentrations, these emissions can have a significant impact on local air quality and visibility reduction, as well as global radiative balance and can also affect cloud and precipitation formation by increasing the number of available cloud nuclei. To better understand wildfire aerosol emissions in the western US, we sampled numerous smoke plumes with a comprehensive suite of aerosol and gas phase instruments onboard the NSF/NCAR C-130 as part of the Western Wildfire Experiment for Cloud Chemistry, Aerosol, Absorption and Nitrogen (WE-CAN) study during the summer of 2018. Here we present aerosol size distributions across a wide diameter range (~10 nm – 3 μm) from combined measurements from a Nano Scanning Mobility Particle Sizer (NSMPS), two Ultra High Sensitivity Aerosol Spectrometers (UHSAS) and a Passive Cavity Aerosol Spectrometer Probe (PCASP). We also present mass and number concentration and mixing state of refractory black carbon (rBC) measured with a Single Particle Soot Photometer (SP2), and concentrations of cloud condensation nuclei (CCN) and derived aerosol hygroscopicity measured with a CCN counter. Overall, wildfire aerosol emissions were found to be dominated by accumulation mode particles, with geometric mean diameters between 150 – 250 nm. Black carbon particles were mostly thickly coated, likely by organic components, and aerosol hygroscopicity was generally very low.

2BC.25

Estimating the Contribution of Significant Volatile Organic Compounds to Secondary Organic Aerosol from Biomass Cookstove Emissions. ADITYA SINHA, Ingrid George, Michael Hays, Andrew Grieshop, *North Carolina State University*

Almost 3 billion people use biomass cookstoves with emissions resulting in adverse impacts on both health and climate. Emissions from these cookstoves include volatile organic compounds (VOCs), which include hazardous pollutants and various precursors to secondary organic aerosol (SOA). However, the identity and extent to which individual VOCs from biomass stove emissions contribute to SOA production is poorly understood. To better constrain VOC identity and quantity for a range of stoves and fuels, we analyzed whole air samples (WAS) of fresh and photochemically-aged emissions using EPA method (TO-15). Using literature yields, we estimate their contribution to SOA observed in an oxidation flow reactor and quantify mass closure in SOA. Preliminary results indicate that Benzene, Naphthalene and Toluene, were capable of explaining up to ~65% of the SOA observed in tests of the most efficient stove, but in other cases only ~10% of SOA formed were explained by these VOCs. On an emission factor basis, the lower combustion efficiency stoves resulted in higher VOCs. SOA contributions from benzene and naphthalene were similar and higher than those from toluene across all conditions. Current work will identify compounds not targeted by the TO-15 protocol, like phenol and derivatives identified as significant SOA precursors, using deconvolution algorithms ('unknowns' analysis) on existing sample analyses. We hypothesize that with the incorporation of VOCs from both targeted and semi-quantitatively estimated non-targeted compounds, we can bridge the gap in unaccounted observed SOA mass. We also explore an alternative approach to explaining the SOA by projecting the VOC measurements from canister sampling, and separate measurements of semi- and intermediate-volatility organic compounds (S/IVOCs) from thermal desorption analysis of collected filters in a volatility basis set (VBS) framework. We will investigate how SOA formation from detailed VOC speciation data compares to estimates applying this VBS framework in explaining observed SOA from cookstove emissions.

2BC.26

Chemical Composition and Morphological Analysis of Internally Mixed Mineral Dust and Biomass Burning Aerosols. JAY TOMLIN, Johannes Weis, Swarup China, Daniel Veghte, Matthew Fraund, Naama Reicher, Quanfu He, Chunlin Li, Yinon Rudich, Ryan Moffet, Mary Gilles, Alexander Laskin, *Purdue University*

In this work, quantitative measurements of particle mixing states were determined in atmospheric particles samples collected in Israel during a Lag Ba'Omer national bonfire festival. Local bonfires spawning across the country yielded significant amount of biomass burning aerosol emitted alongside airborne mineral dust transported from desert areas by regional dust storm. This episode provided unique environmental conditions to allow for the interactions between these two aerosol types. Interactions of mineral dust with biomass burning emissions adds to the complexity of a particles mixing state. We used Computer Controlled Scanning Electron Microscope coupled with elemental microanalysis (Z>Na) to evaluate particle-type population over statistically significant number of particles and Scanning Transmission X-ray Microscopy to examine internal composition of individual particles that allow us to provide quantitative description of particle mixing states. Our findings reveal extensive coating of particle dust components with secondary organic material and present quantitative metrics for practical speciation of aerosol in models.

2BC.27**Optical Characterization of Fresh and Photochemically-Aged Aerosols Emitted from Laboratory Siberian Peat Burning.**

Michealene Iaukea-Lum, Chiranjivi Bhattarai, Deep Sengupta, Vera Samburova, Andrey Khlystov, Adam Watts, W. Patrick Arnott, HANS MOOSMULLER, *Desert Research Institute*

Carbonaceous aerosols emitted by biomass burning greatly influence radiative forcing and climate on regional and global scales. In this study, we characterized the optical properties of emissions from the laboratory combustion of Siberian peat. This fuel frequently burns in large and long-lasting wildland fires affecting boreal and arctic ecosystems. Peat burns mostly in smoldering combustion, emitting large amounts of organic and brown carbon. Here, we characterized the optical properties of both fresh and photochemically-aged emissions. Atmospheric aging was simulated using an Oxidation Flow Reactor (OFR), which was operated with different ultraviolet actinic fluxes to simulate atmospheric aging on timescales ranging from days to months. Aerosol characterization utilized real time instruments including a photoacoustic three-wavelength soot spectrometer (PASS) and a scanning mobility particle sizer (SMPS) with additional analysis of aerosols collected on quartz and Teflon filters. Three-wavelength optical properties of fresh and aged aerosols including single scattering albedo and absorption and scattering Ångström exponents will be presented. In addition, retrieval of complex refractive indices will be discussed.

2BC.28**Polar Fraction of Semi-volatile Organic Compounds in Biomass Burning Emissions and Their Chemical Transformations during Aging with Oxidation Flow Reactor.**

DEEP SENGUPTA, Chiranjivi Bhattarai, Vera Samburova, Adam Watts, Hans Moosmuller, Andrey Khlystov, *Desert Research Institute*

Semi-volatile organic compounds (SVOCs) produced by biomass-burning (BB) contribute to radiative forcing of climate and could also cause adverse health effects. The polar fraction of SVOCs constitutes a significant part of BB organic aerosols and this is why it is important to characterize its chemical composition and reactivity. In the present study, selected representative fuels (both globally and regionally important) were burned under controlled conditions using the DRI chamber facility. Gas and particulate phase biomass burning emissions were aged in an oxidation flow reactor (OFR) to mimic 5-7 days of atmospheric aging. Fresh and OFR-aged biomass-burning aerosols were collected on quartz filters for thermal/optical reflectance (TOR) determination of organic carbon (OC) and on TIGF filters in tandem with XAD resin media for organic compound speciation. TIGF filters and XAD were extracted with a mixture of dichloromethane and acetone. The polar fraction was derivatized prior to GC/MS analysis. 85 polar compounds were quantified including mono and dicarboxylic acids, methoxylated phenols, aromatic acids, anhydrosugars, resin acids and sterols. Carbon content of the quantified polar compounds was found to constitute 2%-5% of the TOR OC. Levoglucosan was found in significant amounts only in Eucalyptus, a representative of flaming combustion type fuels. High abundance of methoxyphenols and resin acids are found in peat burning emissions (smoldering combustion). Concentrations of higher molecular weight compounds decreased after OFR aging, while concentrations of low molecular weight compounds increased. This indicates a significant extent of fragmentation reactions in the OFR. Methoxyphenol concentrations decreased after OFR aging while a significant increase in dicarboxylic acids especially maleic acid was observed. These results can be used to perform source apportionments and predict the processes occurring during atmospheric transport.

2BC.29**Physical, Chemical and Optical Properties of Wildfire**

Aerosols. SWARUP CHINA, Matthew Brege, Simeon Schum, Daniel Veghte, Kaitlyn J. Suski, Gourihar Kulkarni, ManishKumar Shrivastava, Lynn Mazzoleni, Alla Zelenyuk, *Pacific Northwest National Laboratory*

Wildfire is one of the major sources of carbonaceous aerosols in the atmosphere and significantly impacts the radiative forcing of climate at regional and global scales. The radiative forcing of biomass burning aerosol is highly uncertain partly due to the balance between the positive forcing due to absorbing aerosol and negative forcing by weakly absorbing or non-absorbing aerosol particles. Characterization of the physicochemical and optical properties of individual particles and molecular characterization of bulk aerosol are crucial for predictive understanding of radiative forcing of biomass burning particles. Optical properties of biomass burning particles, especially for tar balls, are highly uncertain because of the current knowledge gap about the imaginary part of the complex index of refraction of tar balls. Here, we investigated the physicochemical and optical properties of individual particles from a wildfire influenced plume with high mass loadings. Physicochemical properties of individual particles were characterized using micro-spectroscopy and single particle mass spectrometry techniques and molecular characterization was performed using advanced mass spectrometry techniques. The optical properties of tar balls were derived from the quantitative analysis of the electron energy-loss spectra acquired over individual particles using scanning transmission electron microscopy. A single particle mass spectrometer, miniSPLAT was used to characterize in real-time the size, shape, density, composition, and volatility of individual biomass burning particles. Results indicate that the vast majority of biomass burning particles were spherical tar balls with densities of 1.3 - 1.45 g/cm³, depending on particle size and composition. The characterized particles were nearly non-volatile and retained over 90% of their volume after 24 hours of evaporation at low relative humidity (<5% RH). We will present an overview of the physical, chemical and optical properties of wildfire aerosols. The results from this study should improve predictions of the radiative impact of wildfire aerosols on regional and global climate.

2BC.30**Extreme Molecular Complexity Resulting in a Continuum of Carbonaceous Species in Biomass Burning Tar Balls.**

MATTHEW BREGE, Swarup China, Alla Zelenyuk, Simeon Schum, Lynn Mazzoleni, *Michigan Technological University*

Wildfire aerosol samples heavily influenced by tar balls were collected in the Pacific Northwest to study the detailed molecular properties and address a critical knowledge gap regarding the chemistry of biomass burning tar balls. The organic aerosol extracts were analyzed using ultrahigh resolution Orbitrap Elite mass spectrometry with four complementary ionization techniques. In addition, the physicochemical properties of individual particles were characterized using micro-spectroscopy and single particle mass spectrometry techniques. The resulting data sets contain upwards of 10,000 distinct molecular formulas observed per sample. Each ionization mode had some fraction of exclusive formulas not detected in the other modes, ranging from 2-24% of the total formulas per sample. A majority of the formulas were CHO or CHNO species and were observed in both samples; in addition, a small number of CH, CHN and CHOS formulas were also observed. The overall average O/C ratios were approximately 0.36 with a range of 0-2.3. Many of the molecular formulas appear to be derivatives of polycyclic aromatic hydrocarbons and nitro-phenolic compounds with saturation mass concentrations defined as low or extremely low volatile organic compounds. The estimated dry glass transition temperatures implied that a majority of formulas would be a solid or semi-solid at their respective ambient temperatures. The estimated dry glass transition temperatures increased with molecular weight and the estimated volatilities decreased with molecular weight, consistent with literature expectations. In both of these samples, we observe a continuum of carbonaceous species, which are comprehensive in the observed ranges of oxidation and hydrogen saturation. The observed species span nearly the entire theoretical space of possible molecular formulas for the molecular weight ranges analyzed. This continuum has strong implications for the characterization of organic aerosol, where we expect an exhaustive agglomeration of chemical species to be present at low concentration.

2BC.31**Brown Carbon Formation from Nighttime Chemistry of Unsaturated Heterocyclic Volatile Organic Compounds.**

Huanhuan Jiang, Alexander Frie, Avi Lavi, Jin Chen, Haofei Zhang, Roya Bahreini, YING-HSUAN LIN, *University of California, Riverside*

Nighttime atmospheric processing enhances the formation of brown carbon aerosol (BrC) in biomass burning plumes. Heterocyclic compounds, a group of volatile organic compounds (VOCs) abundant in biomass burning smoke, are possible BrC sources. We investigated the nitrate radical (NO_3)-initiated oxidation of three model heterocyclic VOCs, including pyrrole, furan, and thiophene, as a source of BrC. Utilizing complementary online and offline techniques, we determined the imaginary component of the refractive index at 375 nm (k_{375}), the single scattering albedo at 375 nm (SSA_{375}), and mass absorption coefficients (MAC, 290–700 nm) of the resulting secondary organic aerosol (SOA). Compared to furan and thiophene, NO_3 oxidation of pyrrole has the highest SOA yield. Pyrrole SOA is also more absorbing than furan SOA and thiophene SOA. Compared to other SOA systems, MACs reported in this study are higher than those from biogenic precursors and similar to high- NO_x anthropogenic SOA. High-resolution mass spectrometric measurements revealed unsaturated heterocyclic nitro compounds or organonitrates as possible chromophores in BrC from all three precursors. These findings imply that nighttime oxidation of fire-sourced heterocyclic VOCs, particularly pyrrole, is a plausible source of BrC.

2BC.32**Development of Furan Oxidation Mechanism from OH and NO_3 Oxidation within Biomass-Burning Regimes via Chamber Experiments.** BENJAMIN BROWN-STEINER, Matthew Alvarado, Nga Lee Ng, Taekyu Joo, *AER*

We present the preliminary development of a furan oxidation mechanism within the Aerosol Simulation Program (ASP) based on laboratory chamber experiments at the Georgia Tech Environmental Chamber (GTEC) facility. ASPv2.2 is a young biomass burning plume chemical mechanism that contains over 600 chemical species that merges portions of the MCMv3.2 with portions of RACM2. Furan species found within biomass burning plumes, especially furfural and methylfurans, are quickly oxidized by OH and NO_3 , but there remain many uncertainties as to their oxidation products, their reaction rates, their branching ratios, and their ultimate impact on O_3 and Secondary Organic Aerosols (SOAs). The CTEC chamber experiments, which use a High Resolution Time-of-Flight Chemical Ionization Mass Spectrometer (HR-ToF-CIMS) coupled with a Filter Inlet for Gases and AEROSols (FIGAERO) for the real-time measurement of oxidation products, are designed to determine the furan oxidation products and the O_3 and SOA production under a range of biomass burning chemical regimes by testing different NO_x levels (to simulate different NO_x :VOC ratios), relative humidity, and temperature conditions. We compare the existing ASPv2.2 furan oxidation scheme with a complex NOAA-derived furan oxidation mechanism and, constrained by the results of the chamber experiments, present proposed updates and constrains to the ASP furan oxidation mechanism, as well as potential simplified furan oxidation mechanisms.

2BC.33

Secondary Organic Aerosol Formation from Reaction of 3-Methylfuran with Nitrate Radicals. TAEKYU JOO, Jean Rivera-Rios, Masayuki Takeuchi, Matthew Alvarado, Nga Lee Ng, *Georgia Institute of Technology*

Biomass burning is an important source of both primary and secondary organic aerosol (SOA). Recent studies demonstrate that a large fraction of SOA is produced from nontraditional precursors that are highly reactive to hydroxyl (OH) and nitrate (NO₃) radicals such as furan derivatives. Here, we investigate gas-phase oxidation and SOA formation from 3-methylfuran via NO₃ reaction. Experiments are performed under dry conditions (RH<5%) with different initial concentrations of 3-methylfuran (from 95.9 to 562.8 ppb) at the Georgia Tech Environmental Chamber facility. SOA yield ranges from 1.6 to 2.4% for organic mass loading ranging from 5.1 to 45 μg/m³. More than half of the SOA mass is generated after complete depletion of 3-methylfuran, underlining the importance of higher-generation or heterogeneous reactions to aerosol formation. Particle-phase organic nitrates contribute 39.4% of organics and their volatility (average C* = 10^{-2.9} μg/m³) is higher than that of non-nitrate organic compounds (average C* = 10^{-3.3} μg/m³). A reaction mechanism is proposed based on the compounds that are identified using a Filter Inlet for Gases and AEROSols coupled with time-of-flight chemical ionization mass spectrometer (FIGAERO-HR-ToF-CIMS) and C₅H₅NO₅ and C₅H₆O₃ are determined to be the major species in the gas and particle phases, respectively. Thermogram of particle-phase species suggest that oligomer formation determine the SOA composition and formation rate. Both gas-phase ROOR' formation via RO₂ + RO₂ (acylperoxy radical) reactions and particle-phase accretion reactions can lead to the formation of the dimeric and higher molecular weight compounds. Results from this study can contribute to our understanding of nighttime NO₃ oxidation of furan compounds and aerosol formation in biomass burning plumes.

2BC.34

Emissions, Transport, and Chemistry of Smoke from Western U.S. Wildfires. MEGAN BELA, Natalie Kille, Stuart McKeen, Ravan Ahmadov, Gabriel Pereira, Chris Schmidt, R. Bradley Pierce, Susan O'Neill, Xiaoyang Zhang, Shobha Kondragunta, Christine Wiedinmyer, Rainer Volkamer, *CU CIRES and NOAA ESRL*

Air quality forecasts using regional chemical models provide key information for affected communities and smoke management efforts, yet many models fail to accurately predict ozone (O₃) and particulate matter levels during fire events. The satellite-based emissions and plume rise are large sources of model uncertainty. To improve emissions and plume rise parameterizations, we utilize aircraft and ground-based data from recent field campaigns, such as the 2018 NSF/CU Biomass Burning Fluxes of Trace Gases and Aerosols using SOF on the Wyoming King Air (BB-FLUX) and NSF/CSU Western wildfire Experiment for Cloud chemistry, Aerosol absorption and Nitrogen (WE-CAN) field campaigns, and the 2019 NOAA/NASA Fire Influence on Regional and Global Environments Experiment – Air Quality (FIREX-AQ) field campaign. Hourly fire emissions based on Geostationary Operational Environmental Satellite (GOES)-16/17 fire radiative power are implemented in WRF-Chem. Emission factors (EFs) are updated from estimates from FIREX Fire Lab and BB-FLUX/WE-CAN/FIREX-AQ field observations, and separate EFs are implemented for flaming and smoldering combustion. Uncertainties in emissions and plume injection heights in the model are quantified by comparison with aircraft- and satellite-based estimates. WRF-Chem simulations are also compared with satellite retrievals of trace gases and aerosols, and are used to quantify fire air quality impacts and examine formation/aging mechanisms for O₃ and SOA.

2BC.35

Impacts of Brown Carbon on Surface Shortwave Radiation in the California Sacramento Valley in Summer 2018. CHELSEA CORR, Maosi Chen, Zhibin Sun, Yan'an Liu, George Janson, Becky Olson, Scott Simpson, Amy P. Sullivan, Emily Fischer, Wei Gao, *Colorado State University*

Biomass burning is a significant source of brown carbon (BrC) aerosol which exhibits stronger absorption at ultraviolet (UV) wavelengths ($\lambda < 400\text{nm}$) compared to the visible. The influence of BrC spectral absorption on surface UV and visible irradiance was examined using data collected at the USDA UV-B Monitoring and Research Program's UC Davis site in Summer 2018. Situated in California's Sacramento Valley, the UC Davis site was frequently influenced by wildfire smoke from the large Carr and Mendocino Complex Fires between July and September. Diffuse, direct and total irradiance from two multifilter rotating shadowband radiometers (MFRSRs) at 7 discrete UV wavelengths (300, 305, 311, 317, 325, 332, and 368nm) and 2 visible wavelengths (415 and 500nm) were used to calculate the diffuse fraction of total irradiance (DF) and the diffuse-to-direct ratio (DDR) for cloud-free days before and during the active fire period. Aerosol optical depths (AODs) determined by the Langley method for the UV-MFRSR 368nm channel were used to characterize smoke loading. Measurement-derived DF and DDR values were consistently higher than those modeled for aerosol-free conditions using the Tropospheric Ultraviolet Visible Model (TUV V5.3.2). Further, DF and DDR enhancements in the presence of aerosol increased with AOD, demonstrating the positive relationship between aerosol scattering and diffuse irradiance. Offsets between aerosol-free and measured DDR and DF did show a spectral dependence with largest values at longer wavelengths. This suggests an increase in aerosol absorption relative to scattering as wavelength decreases, a pattern consistent with the presence of BrC. Comparisons between irradiance ratios and measurements of BrC made aboard the NCAR C-130 during the WE-CAN (Western Wildfire Experiment for Cloud Chemistry, Aerosol Absorption and Nitrogen) airborne field campaign were performed to further assess the contribution of BrC to the spectral signatures of the DDR and DF enhancements.

2BC.36

Functional Group Analysis of Wildfire-Influenced Free Tropospheric Organic Aerosol using Ultrahigh Resolution Tandem Mass Spectrometry. SIMEON SCHUM, Claudio Mazzoleni, Bo Zhang, Paulo Fialho, Lynn Mazzoleni, *Michigan Technological University*

A comprehensive ultrahigh resolution tandem mass spectrometry (MS/MS) analysis was performed on wildfire-influenced organic aerosol collected in the free troposphere at the Pico Mountain Observatory. This analysis revealed an unprecedented level of complexity within a single sample of organic aerosol and provided information regarding the polar functional groups present. Using a segmented scanning approach for the analysis of unfragmented precursors, over 9000 individual monoisotopic molecular formulas were identified in the range of m/z 150-500. This represents nearly 4 times more molecular formulas than previously identified within the same mass range using a full scan approach. The increased number of molecular formulas yielded a higher proportion of nitrogen-containing and aromatic molecular formulas. Of the over 9000 identified species, roughly 7000 were observed to have detectable neutral losses representing polar functional groups. The most abundant neutral losses represented carboxyl, hydroxyl, and carbonyl functional groups. Additionally, there were a surprising number of reduced nitrogen and sulfur containing losses as well. The prevalence of carbonyl groups in addition to the reduced nitrogen and sulfur supports a relatively low extent of oxidation for free tropospheric organic aerosol relative to boundary layer organic aerosol. Additionally, the multifunctional nature and isomerization of organic aerosol species is highlighted by the presence of multiple neutral losses for single molecular formulas. Using principal components analysis, neutral losses were attributed to different molecular characteristics (e.g., aromaticity, oxidation, etc.). Thus, novel relationships between neutral loss type and estimated aromaticity were established. This study represents the first comprehensive functional group analysis of organic aerosol using mass spectrometry. The results have implications for molecular structure and modeling studies involving functional groups in aerosol species.

2BC.37

On the Role of NO_x in Biomass Burning Plumes: A Box Model Perspective. QIAOYUN PENG, Brett Palm, Sam Hall, Eric Apel, Rebecca Hornbrook, Alex Jarnot, Nicola Blake, Frank Flocke, Emily Fischer, Joel A. Thornton, *University of Washington, Seattle, WA*

With large primary emissions of nitrogen-containing compounds, important nitrogen chemistry takes place in thick wildfire plumes that impacts the formation of secondary organic and inorganic aerosol. The importance and effects of reactive nitrogen chemistry on biomass burning aerosol evolution were examined using airborne measurements over western U.S. during the Wildfire Experiment for Cloud chemistry, Aerosol absorption and Nitrogen (WE-CAN) Campaign in summer 2018. We employed in situ fresh smoke measurements together with a 0-D photochemical box model to evaluate the extent of NO₃-VOC chemistry compared to OH-initiated oxidation in wildfire plume evolution, as well as SOA formation potential and contribution to inorganic particulate nitrate. With abundant sources of NO₂, O₃, VOCs and sufficiently dark plume center, daytime NO₃-initiated oxidation becomes important due to high NO₃ production rates in young fire smoke, which accelerates the formation of SOA. Our results suggest that neglecting or omitting NO₃ chemistry in photochemical simulations of thick smoke plumes may lead to significant underestimation in the concentration of both organic and inorganic nitrates, which have been observed to form a substantial portion of atmospheric aerosol.

2BC.38

Chemical Composition of Biomass Burning Particles Measured with a Soot Particle Aerosol Mass Spectrometer Downwind during the BBOP Study. TIMOTHY ONASCH, John Shilling, Arthur J. Sedlacek, Edward Fortner, Mikhail Pekour, Shan Zhou, Sonya Collier, Qi Zhang, Andrew Freedman, Leah Williams, Lawrence Kleinman, *Aerodyne Research, Inc.*

The Biomass Burning Observation Project (BBOP), a Department of Energy (DOE) sponsored study, 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.

Chemical signatures reflect different combustion conditions within a given fire plume, indicating 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) changed systematically during the hours of atmospheric transport measured during BBOP. 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.

2BC.39

TD-DFT Investigation of the UV-Vis Spectra of Organonitrogen Chromophores in Brown Carbon. JIN CHEN, Emmy Rodriguez, Huanhuan Jiang, Alexander Frie, Haofei Zhang, Roya Bahreini, Ying-Hsuan Lin, *University of California, Riverside*

Aerosol's radiative forcing is one of the most uncertain drivers of climate cooling and warming. Brown carbon (BrC), light-absorbing organic compounds in aerosols, are estimated to account for ~20% of the tropospheric heating. Recent studies have identified nitroaromatics, conjugated systems, and Maillard reaction products as major BrC chromophores. However, light-absorbing properties of these BrC chromophores from various emission sources (e.g., biomass burning) and precursors have not been fully characterized. This is in part due to incomplete knowledge of their molecular structures and lack of authentic standards. In this study, we investigated the light absorption spectra of organonitrogen compounds as potential BrC chromophores by utilizing computational chemistry approaches. The time-dependent density functional theory (TD-DFT) combined with pure or hybrid functionals (e.g., PBE or B3LYP) was used to compute the excited state molecular geometry and light absorption spectra of tested organonitrogen compounds. In addition, basis sets such as 6-311++G** was incorporated to include diffusion and polarization functions. To explore the solvent effects on the light absorption, the UV-Vis spectra of tested compounds were predicted in gas phase and methanol environment. Calculated UV-Vis spectra were compared with experimental data measured from authentic standards to evaluate the accuracy of our computational predictions accounting for functionals, basis sets and solvent effects. Results from this study will have important implications in identification of potential BrC chromophores and their light absorption properties.

2BC.40

Assessing the Impact of Biomass Burning on Ambient Air Toxics and Ozone Concentration in the Pacific Northwest. ODELLE HADLEY, Anthony Cutler, Ruth Schumaker, Jenna Nelson, Robin Bond, *Olympic Region Clean Air Agency*

The annual use of wood stoves for home heating in Thurston County creates emissions that cause ambient PM_{2.5} to approach, and occasionally exceed, the 24-hour PM_{2.5} National Ambient Air Quality Standard (NAAQS). The seasonal (Oct.-Mar.) PM_{2.5} measured in Thurston County (Lacey) is often equal to, or higher than, measurements in Tacoma and Seattle. In recent years, wildfires caused PM_{2.5} levels to reach unhealthy and very unhealthy levels for several consecutive days. Air samples were collected in Lacey, Washington between August 2018 and July 2019. Eastern Research Group (ERG) analyzed these samples for a suite of toxics, including carbonyls, polyaromatic hydrocarbons (PAH), and volatile organic compounds (VOC). Continuous measurements of PM_{2.5}, black carbon, carbon monoxide and ozone were made coincident with the air toxics sample collection. These air samples represented a wide range of air quality conditions in summer and winter, including days affected by wildfire smoke and emissions from local woodstove and outdoor burning. The chemical profile of air toxics associated with wildfire smoke significantly differed from local wood smoke. The role of meteorology, burn conditions, and smoke source and age are assessed in determining the level of PM_{2.5} toxicity associated with biomass burning.

2BC.41**The Cytotoxicity of Brown Carbon and its Dependence on Combustion Conditions and Light Absorption Properties.**

KHAIRALLAH ATWI, Arnab Mondal, Jitendra Pant, Zezhen Cheng, Omar El Hajj, Hitesh Handa, Rawad Saleh, *University of Georgia*

A large fraction of the organic aerosols emitted from incomplete combustion is light absorbing (henceforth called brown carbon, or BrC). We have previously shown that combustion BrC exhibits a continuum of light-absorption properties that are correlated with the combustion conditions [Saleh et al. (2018) ESTL 5, 8, 508-513]. Here, we build on these findings to investigate the dependence of BrC toxicity on combustion conditions. We used toluene as a model fuel and finely controlled the combustion temperatures and air-to-fuel ratios to produce BrC of different degrees of light absorption, described by the imaginary part of the index of refraction at 550 nm (k_{550}). We collected 3 BrC samples that we categorized as light ($k_{550} = 0.001$), medium ($k_{550} = 0.05$), and dark ($k_{550} = 0.1$). We then analyzed the samples in vitro for their cytotoxicity towards human lung epithelial cells. The procedure involved exposing the cells to 9 doses of each of the BrC samples to determine the dose-dependent cell viability with respect to controls (cells without BrC exposure). We found that the light BrC was cytotoxic (viability < 80%) starting at a dose of 3.7 $\mu\text{g}/\text{cm}^2$, while at a dose of 31.2 $\mu\text{g}/\text{cm}^2$, most cells did not survive, (viability <10%). The medium BrC was only cytotoxic at the highest concentration, 312.5 $\mu\text{g}/\text{cm}^2$ (viability <60%). The dark BrC was not cytotoxic at any dose (viability always >80%). These results suggest that the light BrC emitted from the less efficient combustion, which is typically associated with smoldering combustion conditions, is more harmful to health.

2BC.42**Chamber Studies Investigating Secondary Organic Aerosol Formation and Properties from Daytime and Nighttime Oxidation of Oxygenated Aromatics Emitted by Wildfires.**

CARLEY D. FREDRICKSON, Brett Palm, Amy P. Sullivan, Yingjie Shen, Shane Murphy, Ben H. Lee, Xuan Zhang, Joel A. Thornton, *University of Washington*

We investigated the OH- and NO₃-initiated oxidation of oxygenated aromatics, which included the phenolic compounds phenol, catechol, guaiacol, and cresol in the National Center for Atmospheric Research's 10 m³ Atmospheric Simulation Chamber as part of the Monoterpene and Oxygenated aromatics Oxidation at Night and under LIGHTs (MOONLIGHT) campaign. Using a high-resolution time-of-flight chemical ionization mass spectrometer (HR-ToF-CIMS) coupled with the Filter Inlet for Gases and Aerosols (FIGAERO), we measured the evolution of the molecular composition (O/C, organic nitrogen content, mean molecular weight, etc.) in both the gas and particle phase, together with the corresponding effective volatility of the secondary organic aerosol (SOA) produced in each experiment. We use these observations together with measurements made during the Western Wildfire Experiment for Cloud Chemistry, Aerosol Absorption and Nitrogen (WE-CAN) to constrain the importance of phenolic compounds in the formation of light-absorbing SOA in biomass burning plumes. We also compare the observations to predictions using the FOAM-WAM box model, which uses explicit chemical mechanisms coupled to an equilibrium gas-particle partitioning module, to evaluate the overall skill of known mechanisms and vapor pressure parameterizations at describing SOA from these precursors.

2BC.43

Comparison of Cookstove Emissions and Performance Results Using the Water Boiling Test v4 and the ISO 19867-1 Testing Protocols. WYATT CHAMPION, Craig Williams, Larry Virtaranta, Mark Barnes, James Jetter, *ORISE, U.S. EPA*

Billions of people depend on open fires or simple stoves burning solid fuels each day for cooking. Household air pollution is the world's leading environmental health risk factor and contributes significantly to ambient climate-forcing pollutant emissions. Laboratory testing has typically relied upon the Water Boiling Test (WBT) to both guide practices and allow a unified basis by which to report stove performance and emissions data. In 2018, the International Organization for Standardization (ISO) 19867-1 "Harmonized laboratory test protocols" were released with the intention of establishing improved international comparability for data on air pollutant emissions, efficiency, safety, and durability. The present study compares ISO protocol emissions and efficiency data with WBT data previously collected in the same laboratory (United States Environmental Protection Agency, Research Triangle Park, North Carolina) on the same fuel/stove types (liquefied petroleum gas (LPG), wood pellet, wood fan, wood rocket, wood traditional, and charcoal). On-going data analysis suggests that the ISO protocol results in higher carbon monoxide (CO) and particulate matter (PM) emissions rates/factors for advanced biomass stove types (wood pellet and wood fan) compared to the WBT. The inclusion of both start-up and shutdown periods within each ISO test phase allows stoves to operate at both "steady" and "transitional" conditions and contributes to these higher emission results for these specific stove types (particularly during shutdown). However, when the old ISO International Workshop Agreement (IWA) 11-2012 and the new ISO 19867-3 tier systems for CO/PM emissions are applied to both data sets, cookstove types are similarly ranked (e.g., tier-5 for LPG, tier-4 for wood pellet, tier-0 for wood traditional and charcoal). Therefore, this evaluation of the ISO protocol suggests that it provides data that are both a closer approximation to real-world emissions, and also relatively consistent with former WBT/ISO IWA data in terms of tier ratings for emissions and efficiency.

2CC.1

Aerosol Measurements Using Unmanned Aerosystems. FAN MEI, Darielle Dexheimer, Jason Tomlinson, Mikhail Pekour, Matt Newburn, Albert Mendoza, Casey Longbottom, Lexie Goldberger, Beat Schmid, *Pacific Northwest National Laboratory*

With the increasing deployment of unmanned aerial systems (UAS) and tethered balloon systems (TBS), unmanned aerosystems significantly expand observational perspectives in atmospheric science. The Atmospheric Radiation Measurement (ARM) Aerial Facility (AAF) continues supporting the observation needs of the user community. During a pilot study (PS) at the Southern Great Plains (SGP) atmospheric observatory in July 2019, TBS will be launched with aerosol sensors and meteorology sensors such as iMet radiosondes, fiber optic distributed temperature sensing, and anemometers. Therefore, vertical profiles of the atmospheric state (temperature, humidity, and horizontal wind) and aerosol properties will be observed simultaneously. During a PS in August 2019, a compact aerosol payload will be flying on a group 3 UAS -ArcticShark. Measured aerosol properties include total particle number concentrations, particle size distribution (size range: 135 nm - 1 micron), aerosol absorption coefficient and bulk aerosol chemical composition. Vertical profiles of atmospheric state and aerosol properties will be discussed based on these flights. Changes in the aerosol properties in the boundary layer near the SGP site will also be presented.

2CC.2**Deriving CCN from High-Spectral Resolution Lidar Measurements of Aerosol Extinction and Backscatter.**

RICHARD MOORE, Kyle Dawson, Sharon P. Burton, Snorre Stamnes, Richard Ferrare, Chris Hostetler, Luke Ziemba, Ewan Crosbie, Edward Winstead, Yohei Shinozuka, Kenneth Thornhill, Bruce Anderson, *NASA Langley Research Center*

Airborne field campaigns provide the means to develop and test correlations between CCN number concentrations and remote sensing observations of aerosol optical properties. There have been a number of such assessments in recent years (e.g., Andreae, 2009; Liu et al., 2014; Shinozuka et al., 2015), each with varying degrees of success. Here, we evaluate relationships between aerosol extinction and backscatter coefficients and in situ CCN spectra for a case study in the remote North Atlantic. It is found that in situ measurements reasonably capture aerosol loading on a number basis, but substantially under-sample the coarse mode aerosol that dominate the aerosol optical properties. Methods for unraveling this complexity to remotely sense the submicron aerosol fraction relevant for CCN will be discussed.

2CC.3**Improving Estimates of Ground-Level PM_{2.5} by Application of High Spectral Resolution Lidar.**

XINYI LING, Nicholas Meskhidze, Kyle Dawson, Matthew Johnson, Barron Henderson, Sharon P. Burton, Chris Hostetler, Richard Ferrare, *NC State*

Remote sensing is an effective means of monitoring aerosol properties. Retrievals of aerosol optical depth (AOD) have been used to improve model simulations of PM_{2.5} concentration and to infer ground-level PM_{2.5} over regions where in situ monitoring is not available. However, recent studies have revealed that the AOD-PM_{2.5} relationship can vary from place to place and is strongly affected by aerosol vertical distribution and meteorological variables. Despite advances in active remote-sensing techniques which allow for vertical profiles of aerosol extinction to be used when deriving AOD-PM_{2.5} relationships, current retrievals provide limited information on the chemical composition of aerosols. Here we present a novel approach in which model-predicted concentrations of aerosol chemical species and surface PM_{2.5} are corrected using High Spectral Resolution Lidar (HSRL)-derived vertical extinction and aerosol types. This is achieved by using a new algorithm called Creating Aerosol Types from Chemistry (CATCH). By using this algorithm, the relative contributions of PM_{2.5} chemical components are inferred for measurements acquired during the DISCOVER-AQ Baltimore-Washington, D.C. campaign. The HSRL retrievals of aerosol extinction and types are then used for improving the EPA's CMAQ (Community Multiscale Air Quality) Model simulations of surface PM_{2.5} concentration and chemical composition. The new approach is examined by comparing the data for the prior and posterior CMAQ-predicted aerosol component concentrations and PM_{2.5} with ground measurements from EPA's AQS stations.

Results show an increase in R² values (from 0.30 to 0.65) and reduction of RMSE (from 13.77 to 7.04 µg/m³) for posterior estimates compared with unconstrained simulations. Furthermore, this new methodology allows for the estimation of PM_{2.5} concentration and chemical speciation by using HSRL retrievals of aerosol extinction and types alone. Data derived through the combination of the CATCH algorithm with the HSRL retrievals agree well with ground measurements.

2CC.4

Small Amounts of Alcohol Modify Insoluble Cloud Condensation Nuclei. Farima Barati, Qi YAO, Akua Asa-Awuku, *University of Maryland, College Park*

Organic aerosols and partially soluble particles can uptake water, form droplets and act as Cloud Condensation Nuclei (CCN). Cholesterol is a well-known organic aerosol. Cholesterol is insoluble in water (<0.002 gram in 100 ml of H₂O) but dissolves in organic solvents. In this study, we examine the ability of cholesterol generated in three dilutions of 3 alcohols (ethanol, isopropanol and acetone) to act as CCN. The apparent hygroscopicity, κ , varies over two orders of magnitude, from ~ 0.001 to 0.1. We use statistical analysis of variance (ANOVA) to define significant physical and chemical factors that modify κ . Results show that as volume of water increases, κ changes. However, the type of alcohol does not significantly modify the hygroscopicity. Increases in alcohol concentration decrease droplet surface tension and change aerosol shape. Thus, the apparent κ is corrected with surface tension and shape factor data and estimated to be $\sim 0.028 \pm 0.02$.

2CC.5

Measurements of Removal Rate of Interstitial Aerosols in a Cloudy, Turbulent Environment. ABU SAYEED MD SHAWON, Gregory Kinney, Prasanth Prabhakaran, Jesse C. Anderson, Raymond Shaw, Will Cantrell, *Michigan Technological University*

Aerosol-cloud interactions influence climate by affecting the Earth's radiative budget; they are an uncertainty in assessing anthropogenic effects on climate change. Since aerosols are one of the required ingredients to form cloud droplets, understanding their removal mechanisms is a key aspect to understand this interaction. Forming cloud droplets (activation) becomes the dominant removal mechanism for aerosols that are too big to be highly diffusive and too small to have an appreciable settling velocity. Traditionally, the probability of activation can be described by the chemical composition and the size distribution of the aerosol using the Köhler equation. However, in a turbulent environment, the temperature and water vapor pressure become fluctuating quantities, and so does the saturation ratio. Hence, considering the effects of fluctuating saturation ratio is important in understanding the activation process of an aerosol along with its size and chemical composition.

We investigated this removal mechanism in Michigan Tech's turbulent mixing chamber (also known as the π chamber), where we can create sustained cloud conditions through moist Rayleigh Bénard convection. In steady state conditions, we have measured the size distribution of interstitial aerosols, residual particles (i.e., the particles left after sampling and drying cloud droplets), and cloud droplets. All these experiments suggest that in a turbulent environment, since the saturation ratio fluctuates in time and space, there is no longer a sharp correspondence between the size and activation. Therefore, we have considered a numerical approach to obtain an approximation of the saturation ratio and its fluctuation in a system by using hydrated aerosol and droplet size distribution. We have also explored the relative contributions of aerosol number concentration and chemical composition.

2CC.6**Investigating Different Salt Ions Impact on Cloud Condensation Nucleus (CCN) Activity of Black Carbon Aerosol.**

QI YAO, Howard Fairbrother, Alexa Wallace, Akua Asa-Awuku, *University of Maryland*

Black carbon (BC) particles are emitted into the atmosphere due to incomplete fossil fuel and biomass combustion. BC contributes to lower air quality, atmospheric warming, and regional cloud property modification. However, it is widely known that BC is insoluble and hydrophobic. Thus BC-cloud interactions have not been fully understood; these uncertainties contribute to large uncertainties in net climate prediction forcing from BC sources. Previous research has demonstrated that BC contributes to droplet formation and plays a role as cloud condensation nuclei (CCN) (mostly through models and field sampling experiments). In this study, systematic experiments have been designed to understand the potential impacts from different salt ions (Na⁺, K⁺, Mg²⁺, Cl⁻, SO₄²⁻) on BC aerosol CCN activity. CCN is quantified by the single hygroscopicity parameter (k). Results show that a significant increase in the water-uptake of BC aerosols after mixing with very low (< 0.0001 molar) amounts of salt ions. In addition, different salt ions present varying degrees of contribution to BC aerosol CCN activity growth. This study helps to understand the large hygroscopicity change of BC with the presence of small amounts of salt ions.

2CC.7**Air Mass Characterization for the Megacity Delhi: Impacts on Aerosol Hygroscopicity and CCN Prediction.**

ZAINAB ARUB, Sahil Bhandari, Shahzad Gani, Prashant Soni, Joshua Apte, Lea Hildebrandt Ruiz, Gazala Habib, *Indian Institute of Technology Delhi*

Delhi is a highly polluted megacity influenced by anthropogenic emissions, and this work provides long term, real-time estimates of hygroscopicity parameter ($\Delta\rho$) and CCN. Aerosol composition and size distribution were conducted using ACSM and SMPS respectively at Delhi Aerosol Supersite (DAS) from January, 2017- March, 2018. The 5-days back trajectory revealed three distinct pathways originating from Arabian Sea (AS), Bay of Bengal (BOB) and North-West (NW) regions. The three air masses exhibited distinct characteristics of speciated non-refractory PM₁(NR-PM₁) and size distributions. The NW branch was the most anthropogenically influenced with high organic content and chloride compared to the others. Between the other two, BOB branch was more contaminated than AS branch with a relatively higher organic fraction and nitrate. The average $\Delta\rho$ was approximately 0.3 for all the air masses (0.33±0.06, 0.31±0.06, 0.29±0.06), with strong diurnal variation. The total number concentration, as well as separately for Aitken and Accumulation modes were higher for the air masses originated from NW, followed by BOB and lastly the AS. The predicted CCN concentration and activated fraction (0.7-0.5 at 0.4% SS) for all supersaturations (0.1, 0.4, 0.8) also exhibited the same pattern for the three air masses as for the total number concentration. The CCN concentration showed a more prominent diurnal variation for the north-west compared to other two. On an overall basis, the estimated CCN and activated fractions were higher compared to all Indian measurement sites, which is expected owing to the high pollution occurring both locally and also as transported regionally by the different air masses. The in-depth hygroscopicity measurements are required to make CCN closures accurate and with the knowledge of CCN, cloud droplet number concentration can be better quantified and precipitation by GCMs better understood.

2CC.8

Characterization of Rural Aerosol Hygroscopicity and Chemical Composition Influenced by Fog and Anthropogenic Emissions in Central Taiwan. CHIA-LI CHEN, Ting-Yu Chen, Hui-Ming Hung, Ping-Wen Tsai, Charles C.K. Chou, Wei-Nai Chen, *National Taiwan University*

Ambient submicron particles were investigated using a mini compact time-of-flight aerosol mass spectrometer (mini-c-ToF-AMS), a cloud condensation nuclei counter (CCNc), and a scanning mobility particle sizer (SMPS) from Dec. 1st to Dec. 24th 2018 in the Xitou forest area, Taiwan (23.40°N, 120.47°E, 1,178 m asl). Ambient wet aerosol particles were collected by a 13-stage nano-MOUDI II impactor (micro-orifice uniform deposit impactors) and post-analyzed by a Fourier-transform infrared spectroscopy (FTIR). This study investigates the influence of meteorological and geographical conditions (e.g., sea/land breeze circulation, upslope fog formation, and mountain-valley breezes) on chemical composition of non-refractory submicron particles and single hygroscopicity parameter (κ) of particles at Xitou. Organics (62%), sulfate (22%), and nitrate (6%) concentrations correlate moderately with chloride, suggesting the aerosol particles are likely northwesterly transported from coastal areas (a distance of 60~70 km) by sea breeze. The late afternoon (16:00-17:00) peak of aerosol particles is likely due to slow transport of 60-km industrialized pollutants from a coastal power plant and chemical plants by daytime sea breeze or valley breeze and combination of secondary organic aerosol formation. The κ ranges of sulfate particles derived from AMS particle time-of-flight (ptof) and FTIR measurement comparisons are $0.2 < \kappa < 0.5$ and $0.6 < \kappa < 0.8$ during daytime on foggy days and non-foggy days, respectively. The high relative humidity range of 95% to 99% could likely promote the process of cloud droplets activation during nighttime, thus the derived κ value ranges of sulfate particles are lower than 0.4. This study will investigate the κ profile as a function of aerosol size derived from AMS-SMPS/AMS-FTIR and CCNc measurement and the impact of the upper stream anthropogenic emissions on the aerosol physical-chemical properties over the rural areas.

2CC.9

Simulation of Air Pollution and Its Meteorological Feedbacks in Africa. PENGFEI WANG, Hao Guo, Yuan Wang, Peng Wang, Qi Ying, Hongliang Zhang, *Louisiana State University*

In recent years, air pollution problems happened globally, especially where has a large population and rapid economic development resulting in large anthropogenic emission. Africa is now under this circumstance yet studies on air pollution are limited particularly of the whole continent. In this study, simulation of air pollutants like particulate matter and ozone over the whole continent of Africa at 36-km grid resolution was conducted for dry and rainy season in the year of 2015 by using Weather Research and Forecasting model coupled with Chemistry (WRF/chem). Model performance will be validated by comparing meteorological observations and air pollutants. By comparing the prediction results generated by WRF/chem model with the observation results from the NASA earth science data such as Multi-angle Imaging SpectroRadiometer (MISR), Moderate Resolution Imaging Spectroradiometer (MODIS), and Aerosol Robotic Net- work (AERONET) aerosol optical depth (AOD) products, the performance of WRF/chem model will be validated. The seasonal and spatial variation in concentrations of pollutants including particulate matter and ozone will be analyzed and associated with meteorological changes like temperature, wind, precipitation, mixing layer height, and relative humidity. The impact of the direct effect of aerosol particles on radiation and the indirect aerosol effect on meteorological variables and subsequent distributions of particulate matter and ozone will also be investigated. The differences between meteorological feedbacks during dry and rainy seasons will be compared. This study would provide information for evaluating WRF/chem model performance and meteorological feedbacks for Africa and the basis for future source apportionment and health-related studies.

2CC.10

Contribution of Particulate Matter Components to Hydroxyl Radical Formation by Aerosols in Simulated Cloud Water and High Activity Associated with Biomass Burning Aerosol. Xiaobi M. Kuang, David Gonzalez, J. Adlin Scott, Kennedy Vu, Tiffany Charbouillot, Alam Hasson, Lelia Hawkins, SUZANNE E. PAULSON, *UCLA*

Hydroxyl radical (OH) reactions in cloud water play a key role in secondary organic aerosol formation and sulfur oxidation. We collected aerosol samples (PM₄) at an urban receptor site in Claremont, California during summer and at a site in Fresno, California with substantial biomass burning aerosol during winter. The Claremont site mostly receives air from the urban area in the morning, photochemically processed air arriving from the urban area and a commercial ports area in the afternoon, and a largely unpopulated mountainous area overnight. Filters were extracted in small quantities of water at pH 3.5, simulating cloud water formation. Samples were analyzed for particle mass, OH generation in the presence of near UV light, soluble trace metals (filtered through a 0.22 μm filter, measured with inductively coupled plasma mass spectrometry, ICP), soluble Fe(II) and Fe(III) (measured with the ferrozine assay, Fefzn), quinones and biomass burning aerosol (BBA) content. For Claremont, soluble speciated iron was about equally divided into Fe(II)fzn and Fe(III)fzn, and accounted for only 22 ± 7 % of the soluble FeICP. For Fresno, Fefzn was mostly in its reduced form. The highest concentrations of Fefzn came from the urban area; high FeICP came both from city and mountains and the mountains were the dominant source of Cu. OH formation was characterized by an initial spike in formation lasting for 1-3 minutes with a formation rate of $\sim (0.2 - 1) \times 10^{-8} \text{ M} \times \text{s}^{-1}$, followed by a second much slower phase of $(0.1 - 10) \times 10^{-11} \text{ M} \times \text{s}^{-1}$. OH formation activity was strongly correlated with mass and soluble (ICP) Fe and Cu; it did not correlate with ferrozine iron. Fresno samples containing biomass burning aerosol produced far more OH than any other samples, and a multivariate linear regression showed that a combination iron, manganese and BBA were the most significant contributors to OH formation, with $r^2 > 0.9$. The initial burst of OH formation is large enough to contribute substantial OH to cloud and fog drops.

2CC.15

Predicting the Phase State of Secondary Organic Aerosol and Understanding its Influences on the Heterogeneous Ice Nucleation. YUE ZHANG, Martin Wolf, Shachi Katira, Jason Injae Jung, Abigail Koss, Peyton Spencer, Xiaoli Shen, Andrew Lee, Andrew Lambe, Wen Xu, Leonid Nichman, Yuzhi Chen, Manjula Canagaratna, Zhenfa Zhang, Avram Gold, John Jayne, Douglas Worsnop, Paul Davidovits, David Chandler, Timothy Onasch, Charles Kolb, Jesse Kroll, Jason Surratt, Daniel Cziczo, *Univ. of North Carolina, Chapel Hill/Aerodyne Research, Inc.*

Particulate matter (PM) has important effects on the climate, human health, and visibility. 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 have important implications for reactivity, growth, and cloud formation capabilities of organic aerosols (OA), and is also an important constraint for estimating aerosol viscosity.

The glass transition temperatures (T_g) of selected organic components and organic-organic binary mixtures were measured at selected atmospherically relevant cooling rates (2-10 K/min). The results indicate that increasing the cooling rate can reduce the glass transition temperatures of organic compounds by 4-5 K, leading aerosol becoming glassy 400-800 meter lower in the ambient atmosphere than the base condition. A semi-empirical relationship between the glass transition temperatures and aerosol volatility is also established through experimental measurements and modeling, facilitating parameterization of aerosol viscosity and phase state into regional and global models.

Given that in the free troposphere OAs can exist in semi-solid or solid phase states, such transition of the phase state may potentially increase the heterogeneous IN activity. A laboratory study was systematically performed to examine the effects of aerosol-phase state on heterogeneous IN properties of OAs by using the spectrometer for ice nucleation (SPIN), a commercially available instrument (Droplet Measurement Technologies, Inc), potential aerosol mass (PAM) oxidation flow reactor, and the MIT environmental chamber.

OAs comprised of representative surrogates and the actual secondary organic aerosols (SOA) from various precursors were generated and passed through a temperature control apparatus, where the temperature of the aerosols was kept between -45~20°C before entering the SPIN. Our results show that certain pre-cooling the aerosol particles enhances the IN onset relative humidity (RH) and the active fraction of IN. Coupled with viscosity and glass transition temperature calculations, the aerosol phase state changes is shown to be the reason for the enhanced ice nucleation, however the chemical composition of the aerosols also have important influences on the IN properties.

2HA.1

Oxidative Potential and Cytotoxicity of Ambient Fine Particulate Matter During Winter at Beijing, China and Gwangju, Korea. Ma. Cristine Faye Denna, Lucille Joanna Borlaza, Hangyul Song, Enrique Cosep, ILHWA SEO, Hyunok Maeng, Minhan Park, Min-Suk Bae, Kihong Park, *Gwangju Institute of Science and Technology*

Ambient fine particulate matter less than $2.5\mu\text{m}$ ($\text{PM}_{2.5}$) has gained concern due to its harmful health effects, especially in East Asian countries. In this study, simultaneous measurement of ambient $\text{PM}_{2.5}$ in Beijing, China and Gwangju, Korea was conducted during winter (01.03.2018 – 02.01.2018). Samples were characterized by their chemical properties (ions, elements, and organic and elemental carbon) and their toxicity was assessed by measuring oxidative potential and cytotoxicity. Oxidative potential, the capability of $\text{PM}_{2.5}$ to produce reactive oxygen species which can damage the cells, was measured using dithiothreitol (DTT) assay. Cytotoxicity was analyzed with neutral red uptake (NRU) assay using epithelial lung cells that were exposed to $\text{PM}_{2.5}$ extracts. Average $\text{PM}_{2.5}$ mass concentration in Beijing was higher than Gwangju with values of $62.45\ \mu\text{g}/\text{m}^3$ and $26.77\ \mu\text{g}/\text{m}^3$, respectively. The contribution of chemical composition for the two sites was also distinct: Beijing (elements (35.9%) > carbonaceous species (OC/EC) (27.9%) > ions (21.7%)) and Gwangju (ions (49.6%) > carbonaceous species (OC/EC) (20.4%) > elements (10.9%)). The average values for the mass- and volume-normalized OP activity (OP-DTT_m and OP-DTT_v , respectively) were found to be larger in Beijing than Gwangju (OP-DTT_m : $53.38\ \text{pmol}/\text{min}/\mu\text{g}$ vs. $44.27\ \text{pmol}/\text{min}/\mu\text{g}$ and OP-DTT_v : $2.48\ \text{nmol}/\text{min}/\text{m}^3$ vs. $1.13\ \text{nmol}/\text{min}/\text{m}^3$, respectively). The difference in OP-DTT_m for both sites was not as high compared to the difference in the $\text{PM}_{2.5}$ mass concentration. The OP-DTT_m values for event cases were almost the same in both sites (Beijing: $55.58\ \text{pmol}/\text{min}/\mu\text{g}$ and Gwangju: $57.91\ \text{pmol}/\text{min}/\mu\text{g}$) while OP-DTT_v values increased by a factor of 2.5 and 3 for Beijing and Gwangju, respectively, in event days compared to the average values. Cytotoxicity was also determined for the samples from Gwangju where the lowest cell viability was observed with the highest $\text{PM}_{2.5}$ mass concentration. Similar trends were observed for cytotoxicity and OP-DTT in event days but this was not observed for non-event cases. Comprehensive measurement of aerosol effects can be obtained using cytotoxicity analysis, and comparing it with a chemical assay would support the identification of ROS production mechanism and PM components causing aerosol health effects. To further characterize the different factors affecting the OP activity and cytotoxicity and their relationship, the effect of chemical properties of $\text{PM}_{2.5}$ will also be investigated.

2HA.2

Particle Size and Concentration of Aerosols Produced by Electronic Nicotine Delivery Systems. SHERRIE ELZEY, Andrea Tiwari, Jon Ebbert, Slobodan Macura, *TSI Incorporated*

The particle size of inhaled aerosols can be correlated to lung deposition, with smaller sizes penetrating into deeper regions of the lung. Thus, time-resolved particle size and concentration data can be used to approximate the dosing rate of chemical substances inhaled from electronic nicotine delivery systems (ENDS). The objective of this study was to measure the particle size distribution (PSD) of aerosols produced by different types of ENDS and e-liquids. A smoking machine was used to control the puff profile and deliver a repeatable puff volume. ENDS aerosols were characterized using an Engine Exhaust Particle Sizer to capture nanoscale particles from 5 – 560 nm and an Optical Particle Sizer to capture microscale particles from 0.3 – 10 μm . Diluters were used upstream of the sizers to ensure that concentrations were within measurement limits. PSDs were collected at an acquisition rate of 10 Hz to observe temporal changes, in addition to mean particle size and average total concentration. Results show that rapid changes occurred in the PSDs in terms of both particle size and concentration. These results indicate that 1) PSD data can be used to approximate the dosing rate for a smoker and categorize ENDS or e-liquids as comparatively more or less hazardous; and 2) fast-response sizing techniques provide a comprehensive characterization of PSDs that includes time evolution.

2HA.3

Field and Laboratory Measurements of Aerosolized Blue-Green Algal Toxins in South Florida. MICHAEL SHERIDAN, Haley Plaas, Haley Royer, Lilly Blume, Chuyan Wan, Dhruv Mitroo, Kimberly Pependorf, Larry Brand, Cassandra Gaston, *University of Miami*

Cyanobacteria (e.g., blue-green algae) form Harmful Algal Blooms (HABs) in freshwater lakes and produce several toxins, most notably β -N-methylamino-L-alanine (BMAA) and microcystin. These toxins present a public health concern, since microcystin has been found to promote liver cancer while BMAA has been recognized as a neurotoxin correlated to neurodegenerative diseases including Alzheimer's disease, Parkinson's disease, and Amyotrophic Lateral Sclerosis (ALS). The impact of BMAA and microcystin on seafood and water quality have been investigated, but the more direct exposure route through toxin-containing inhalable particles has not been well-established. In the summer of 2018, a massive bloom of cyanobacteria adversely impacted South Florida's lakes, rivers, canals, and lochs. We collected air samples near these waterways and lake water samples that we used to generate lake spray aerosol with a bubbling apparatus. The aim of this work is to quantify aerosolized BMAA and microcystin concentrations in ambient air and water samples and in aerosols generated from bubbled water samples as well as to determine the water-to-air transfer of these toxic compounds. We measured BMAA and microcystin concentrations in both ambient and lab-bubbled air and in water samples using standard methods (e.g., enzyme-linked immunosorbent assay (ELISA)) and mass spectrometry methods capable of quantifying individual toxin congeners. Our analysis shows that toxins are indeed aerosolized, which has implications for how blue-green algae blooms can impact air quality and health in South Florida.

2HA.6

The Influence of Temperature on Microcystin Concentration in Bubble-Generated Lake Spray Aerosols. HALEY PLAAS, Kimberly Pependorf, Cassandra Gaston, Larry Brand, *University of Miami*

Cyanobacteria, or blue-green algae, are planktonic phototrophs that flourish in aquatic environments of every continent. Under eutrophic conditions, cyanobacteria can dominate as dense blooms, negatively impacting water quality. Anthropogenic activity, such as nutrient-loading and climate change, have been demonstrated to intensify cyanobacterial blooms in recent decades. Harmful cyanobacterial blooms (CyanoHABs) are particularly problematic as several genera produce toxins, some including microcystin, a known hepatotoxin. While numerous studies regarding CyanoHABs have investigated the consumption of contaminated food stuffs or water, little research has been conducted to assess the health risks of exposure to cyanotoxins found in aerosols. This study quantified microcystin in bubble-generated lake spray aerosol and investigated the influence of increased water temperatures on the aerosolization of microcystin. Cyanobacteria samples were collected from Lake Okeechobee, Florida during bloom episodes that occurred in the late summer of 2018, then maintained in culture. To simulate the bursting of primary aerosols at the lake-air interface, dilute culture was placed in a bubbling apparatus and resultant aerosols were collected on a filter. Three temperature treatments were chosen to investigate the relationship between water temperature and microcystin concentration in aerosols: room temperature (23C), a typical summer lake surface temperature in Lake Okeechobee (30C), and an elevated lake surface temperature based upon projected climate models (31.5C). Each treatment was run in triplicate on three separate trial days. There is no statistical evidence presented to suggest that temperature plays a role in altering the concentration of aerosolized microcystin compounds. Interestingly, we did not observe a consistent relationship between chlorophyll concentration and microcystin concentration in the water or aerosols. However, this pilot study confirms the ability of microcystin to become airborne and highlights the potential of respiratory exposure to microcystin, along with other cyanotoxins, as a worthy public health concern.

2HA.7

The Characterization of Emissions from Sawing and Sanding Corian[®], a Solid-Surface Composite Material. Seungkoo Kang, CHAOLONG QI, *NIOSH*

We conducted laboratory tests to characterize composition of emissions from sawing and sanding Corian[®], a solid surface composite material composed of acrylic polymer and alumina trihydrate (ATH). The test system enables automatic sawing and sanding of Corian[®] board repeatedly in an enclosed chamber and taking representative air samples in a duct downstream of the chamber. The air samples were analyzed for both dust containing metal element contents (especially aluminum) and volatile organic compounds (VOCs). Three different sanding belts (ceramic, silicon carbide, and aluminum oxide with 120 grit) were tested to distinguish the contribution of aluminum-containing dust in the emission from Corian[®] and sanding belt itself. Airborne dust samples were collected using a Micro-Orifice Uniform Deposit Impactor (MOUDI), and the aluminum content of size-classified dust samples were analyzed. The analyses also included semivolatile organic compounds (SVOCs) in bulk and respirable dust samples as well as volatile organic compounds (VOCs) samples in the emission. The normalized respirable dust generation rate from MOUDI was 5.9, 24.0, 31.8, and 20.1 milligrams per gram (mg g⁻¹) from sawing, sanding with silicone carbide, ceramic, and aluminum oxide, respectively, indicating that more dust became respirable during sanding. The ATH content of the dust was above 80% in most parts of the respirable size range from both sawing and sanding with all three types of sanding belts, suggesting that ATH is the dominant composition of the respirable dust and ATH was dominantly generated by Corian[®]. Finally, a small amount of methyl methacrylate (MMA) (0.55%) was found in the bulk dust but not in the respirable dust from the SVOC analysis. VOC analyses revealed that MMA was the most abundant compound in the vapor form, resulting in 0.0069% of the mass removed from sawing Corian[®] became MMA vapor. 0.0026%, 0.0028%, and 0.0022% of the mass removed from sanding Corian[®] became MMA vapor with ceramic, silicon carbide, and aluminum oxide belts, respectively, suggesting a lower generation rate of VOCs in sanding compared to sawing Corian[®].

2HA.8

Quantification of OH Radicals Generated by Secondary Organic Aerosols with Fluorometric Assay and Electron Paramagnetic Resonance Spectrometry. JINLAI WEI, Ting Fang, Manabu Shiraiwa, *University of California, Irvine*

The adverse health effects of ambient particulate matter (PM) are linked to the oxidative potential, known as the capability to generate reactive oxygen species (ROS) in vivo. Secondary organic aerosols (SOA) account for a large fraction of ambient PM, but the mechanisms of SOA inducing ROS generation are not well understood. Hydroxyl radicals are of great concern among ROS due to their drastic effects on biological tissues and cell components. Various acellular techniques have been applied for the quantification of OH, among which the fluorometric assay is most widely used. Electron paramagnetic resonance (EPR) spectrometry coupled with a spin trapping technique has also been used for OH measurements, which also enables simultaneous detection of other radical species including superoxide and organic radicals. However, the applications of these techniques have not been compared in measuring OH, and their pros and cons have not been well discussed. In this study, we investigated the hydroxyl radical generation from Fenton reaction using both fluorometric assay and EPR with spin trapping. Despite the difference in OH concentrations measured by the two methods, the kinetic modeling revealed a good agreement in OH production rate. Our preliminary results show that it is necessary to couple kinetic modeling with experimental techniques when bridging different methods in ROS measurement to exclude the impacts of associated artifacts. We plan to further investigate the ROS activity of laboratory-generated SOA from biogenic, anthropogenic and indoor-relevant precursors, and their interactions with transition metals using both techniques combined with kinetic modeling.

2HA.9

Impacts of Adding Dispersant on Aerosolization of Fine and Ultrafine Particulate Matter after an Oil Spill. NIMA AFSHAR-MOHAJER, Lakshmana Dora, Andres Lam, Ana Rule, Joseph Katz, Kirsten Koehler, *Johns Hopkins School of Public Health*

Bubble bursting of oceanic whitecaps is a primary source of marine aerosol emission. After an oil spill, inhalation of the fine PM containing toxic petrochemical compounds, emitted due to bubble bursting, cause serious pulmonary diseases to cleanup workers and nearby inhalers. Spraying chemical dispersants to enhance distribution of the crude oil into the water was employed extensively during the Deepwater Horizon spill. However, our previous work has shown an increase in fine PM with use of chemical dispersants. Risk assessment of such exposure requires information about the chemical composition of the airborne PM. In this study, we determined the chemical constituents of the fine PM (PM_{2.5}) and ultrafine PM (UFPs) emitted from seawater covered with a crude oil (MC252 surrogate) slick of 0.5 mm, before and after mixing with dispersant (Corexit 9500A, dispersant to oil ratio of 1:25 Vol./Vol.). Aerosol generation was facilitated through the bursting of air bubbles injected at controlled diameter of 0.6 mm into a vertical seawater column (L=0.3, W=0.3, and H=0.6 m), the bubbles rise to the oil-contaminated water surface and burst. The resulting aerosols were sampled onto 37-mm quartz filters using a Personal Environmental Monitor (PEM) for PM_{2.5} and a filter/cassette for total suspended particles with and without presence of dispersant. Using Pentane as solvent, PM were extracted from the filters, then analyzed for composition via a gas chromatography/mass spectrometry system. Primary tests confirmed demonstrated that dodecane and 1-(2-butoxy-1-methylethoxy)-2-propanol (BMEP) are the best identifiers for crude oil and dispersant, respectively. The crude oil marker of dodecane exists in PM_{2.5} filters obtained from the experiments with seawater polluted by the mixture slick. As an indicator for increase in concentration of the finer PM, the dodecane content of the TSP filters reduced 19.2% (61.2 to 49.4 µg/mL) when dispersant was the sprayed, but the dodecane content of the PM_{2.5} increased 7.4% (33.4 to 35.6 µg/mL). Furthermore, a 12-stage low-pressure cascade impactor (LPCI) collected the particles with size bins to be with cut off diameters of 9.5, 6.2, 4.2, 2.9, 1.8, 0.95, 0.51, 0.38, 0.30, 0.20, 0.13, and 0.056 µm onto 81-mm filters. Both dodecane and BMEP were detected on the filters collected from multiple stages of the LPCI. Changes in dodecane contents at each stage compared to the case without dispersant, and anticipated health impacts will also be presented.

2HA.10

Aerosol Size Distribution and Aldehyde Concentration Measurements of the Sub-ohm Electronic Nicotine Delivery Systems. VLADIMIR MIKHEEV, Stephanie S. Buehler, Alexander Ivanov, *Battelle Memorial Institute*

Electronic nicotine delivery systems (ENDS) are considered as a safer alternative to the combustible tobacco smoking but actual level of the harmful and potentially harmful constituents (HPHC) emitted by ENDS remains unclear. Newest ENDS with electrically heated coil resistance less than one ohm (sub-ohm) can be used at heating power level up to ~200 W that significantly exceeds earlier types of electronic cigarettes. Characterization of both physical (aerosol size distribution) and chemical properties of the aerosol generated by sub-ohm ENDS is urgently needed to assess harmful risk of these devices.

Sub-ohm ENDS were used to generate aerosol out of propylene glycol and glycerol 50/50 mixture at a wide range of heating power level (from 10 to 150 W) and at the various puffing flow rates (10 – 70 mL/s). Aerosol size distribution was analyzed using differential mobility spectrometer (DMS500) and Electrical Low Pressure Impactor (ELPI). Aldehydes concentration was measured using Proton-Transfer Reaction Quadrupole Mass-Spectrometer (PTR-QMS). Total particulate mass (TPM) was defined by taking gravimetric analysis of the aerosol deposited on the quartz-fiber filters.

Particles of larger size (than was previously measured for the first generation of e-cigarettes) was observed (mass median aerodynamic diameter ~1 micron). High concentration of aldehydes (formaldehyde, acetaldehyde, and acrolein) exceeding the level previously measured for the earlier types of e-cigarettes was detected (starting from 50 W heating power and higher). TPM has exceeded 50 mg/puff. High concentration of HPHCs (formaldehyde, acetaldehyde, and acrolein) detected in sub-ohm ENDS emissions increases health concerns associated with vaping of these devices.

2HA.12

Real-Time Chemical Puff Profiling of Vapor Product Aerosol with Proton Transfer Mass Spectrometry. Adam M. Ozvald, Devon C. O'Regan, Alessandra L. Paul, NADJA HEINE, *Juul Labs, Inc.*

The analysis of aerosol and gas phase volatile organic compounds (VOC) emitted by vapor products has relied on a variety of standardized but time-consuming off-line technologies. Conventional methods typically involve the capture of aerosol from multiple sequential puffs (~50) on a filter pad, or in an impinger solution, followed by extraction and derivatization. These procedures are resource intensive and have low time-resolution, prohibiting puff-by-puff analysis, and may lead to sample alteration due to evaporation, water uptake, or chemical reactions on the filter. Real-time aerosol and VOC characterization methods can overcome these limitations and enable the direct assessment of multiple key components simultaneously. Recently, Breiev *et al.*¹ demonstrated that proton transfer reaction mass spectrometry (PTR-MS) can be employed to achieve on-line quantification of the three main components of aerosol emitted from vapor products.

In this study, we present a novel methodology which combines a high-resolution PTR-MS with an improved aerosol dilution system and an actuating device to trigger aerosol production from the vapor product and direct it to the dilution system. We employed this methodology to analyze and quantify harmful or potentially harmful constituents (HPHCs) in aerosol emitted from vapor products and exhaled breath on a puff-by-puff basis in real-time.

The methodology was evaluated for applicability and stability in order to perform reliable, real-time quantification of HPHCs as well as to examine conditional use scenarios, such as the chemical puff profile at the end of battery or liquid supply. Key aerosol and VOC constituents of vapor products were directly and simultaneously characterized and quantified, and their LODs assessed and compared to standard offline methods. Concentrations of several compounds were determined puff-by-puff and validated with results obtained from a contract research laboratory using ISO 17025 accredited methods. The chemical puff profiles of different devices (e.g. temperature-regulated, unregulated, and ciga-likes) are presented. The real-time data demonstrates that harmful compounds were not detected for temperature regulated devices for the life of the pod, while in contrast, devices without temperature regulation exhibited significant increase of harmful compounds such as carbonyls and oxides at the end of liquid.

Lastly, we compared exhaled breath following the inhalation of mainstream aerosol from different vapor products and a combustible cigarette. We demonstrate that PTR-MS may be used as an alternative to off-line methods for simultaneous quantification and characterization of most HPHCs found in aerosol as well as VOCs, puff-by-puff, and even intra-puff to enable immediate assessment of new nicotine-containing formulations, changes in device design, and validation of product designs.

[1] K. Breiev *et al.*, *Rapid Commun. Mass Spectrom.* **2016**, 30, 691.

2HA.14

Understanding the Glottis Motion Effect on Aerosol Transport and Deposition in a Subject-Specific Human Upper Airway Configuration. JIANAN ZHAO, Yu Feng, *Oklahoma State University*

To precisely estimate the lung uptake of airborne toxic particles with different exposure conditions for health risk assessment, high-resolution data on how they transport and deposit in human respiratory systems are critically needed. Computational Fluid-Particle Dynamics (CFPD) models have been employed for such studies for decades. However, existing CFPD models assume the glottis is static during the breathing cycle. Indeed, glottis has the narrowest passage and generates a laryngeal jet and recirculation of airflows downstream in the trachea. The transient glottis motion, i.e., adduction and abduction within the breathing cycles, could enhance the pulmonary airflow unsteadiness and the resultant inhaled particle deposition, which have not been well studied. Therefore, a novel CFPD model was developed in this study with the capability of modeling the glottis motion using dynamic mesh. To explore the causal relationships between the glottis motion and the aerosol dynamics in a subject-specific upper airway model, simulations were performed with both rigid and dynamic glottises in a sinusoidal breathing cycle representing the resting condition. The glottis adduction and abduction were achieved by controlling the movement of each node of the dynamic mesh, which is validated by clinical data. Specifically, 45,236 particles were inhaled with their diameters equal to 0.5 microns. Numerical results indicate that the realistic glottis motion induces more particles passing through the throat and entering the tracheobronchial region. Numerical deposition results indicate that the glottis motion leads to airflow pattern variations compared with the rigid glottis setup. Subsequently, glottis motion generates lower DFs in the oral cavity, oropharynx, and larynx, but slightly higher DF in the glottis. Glottis adduction during exhalation results in more particle depositions than the rigid glottis case. In conclusion, the glottis motion shows significant influence on particle deposition predictions and must be considered in CFPD simulations in the future.

2HA.17

Characterization and Performance Evaluation of a Nose-only Inhalation (NOI) Exposure System for a 90-Day Repeated-Dose NNK Inhalation Toxicity Study. Shu-Chieh Hu, Yunan Tang, Seonggi Min, Hyun-Ki Kang, Dong-Jin Yang, Mallikarjuna Basavarajappa, Estatira Sepehr, Raul Trbojevich, Matthew Bryant, JINGHAI YI, Susan Chemerynski, Steven Yee, Hans Rosenfeldt, R. Philip Yeager, Paul Howard, *NCTR-FDA*

Human exposure to 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK), a tobacco-specific nitrosamine classified as a carcinogen, occurs through the use of combusted or smokeless tobacco products, or exposure to environmental tobacco smoke. However, studies of inhaled NNK are limited. To properly perform a 90-day inhalation toxicology study, aerosols in NOI chamber must have (1) a steady mass concentration maintained at a desired level for the entire exposure period, (2) a stable size distribution with a mass-median-aerodynamic-diameter (MMAD) < 2 μm and a geometric-standard-deviation (GSD) of 1 to 3, (3) a spatially-uniform distribution, and (4) a repeatable concentration. To date, no method has been reported on generating respirable NNK aerosols with a stable and repeatable concentration. Six NOI exposure systems were characterized in a 90-day NNK inhalation toxicology study. Each system consisted of (1) an aerosol generation system, (2) a 50-port NOI exposure chamber, and (3) a test atmosphere control and monitor system. NNK aerosols, generated from NNK formulation (NNK dissolved in propylene glycol and water) with a nebulizer, were delivered into the NOI exposure system at 50 LPM. Particle size distribution was measured using a cascade impactor. NNK concentration was determined by gravimetric collection of aerosols into filter and analyzed by an ultra-high-performance-liquid-chromatography. The air pressure, temperature, relative humidity, and oxygen concentration were monitored and controlled continuously. The NNK aerosols delivered to the NOI exposure systems had (1) a steady concentration at 0.0066, 0.026 and 0.257 mg/L during a 1-hour exposure, (2) a stable size distribution with a MMAD of 1.21~1.77 μm and a GSD of 1.55~2.0, (3) a spatially uniform distribution with a spatial variation < 3%, and (4) a repeatable concentration with a relative-standard-deviation < 5.0%. The six nose-only inhalation exposure systems reliably and repeatedly created well-controlled test atmospheres that can be used to evaluate the health impact of NNK inhalation exposures.

2HA.20

Development and Comparison of Complementary Methods to Study Skin and Inhalational Exposure to Simulant Pathogens During Personal Protective Equipment Doffing.

JENNIFER THERKORN, David Drewry, Jennifer Andonian, Lauren Benishek, Carrie Billman, Ellen Forsyth, Brian Garibaldi, Elaine Nowakowski, Kaitlin Rainwater-Lovett, Lauren Sauer, Maggie Schiffhauer, Lisa Maragakis, *Johns Hopkins University Applied Physics Laboratory*

There is much concern regarding the potential for healthcare workers to become exposed to pathogens while wearing/doffing personal protective equipment (PPE) after caring for patients with high consequence pathogens. Fluorescent tracers are often used in PPE studies with ultraviolet lights to identify where healthcare workers contaminate themselves during doffing. This method is limited in detection sensitivity to what can be seen by the human eye and airborne contamination in subjects' breathing zones cannot be detected. To address these issues, a method was developed using 2 μm polystyrene latex spheres (PSLs). Study participants (n=5) were contaminated with both the traditional fluorescent tracer and nebulized PSLs while following the CDC recommended guidelines for PPE to care for patients with high consequence pathogens. Skin contamination was investigated by UV light for the fluorescent tracer, and via swabbing for PSLs. Potential inhalational exposure of PSLs was determined with a breathing zone air sampler (Button Sampler). In the pilot study, all study subjects had PSL and fluorescent tracer skin contamination. Two subjects had simultaneously-located contamination of both types on a wrist and hand. For all other subjects, the PSL method showed skin contamination that was not detected by the fluorescent tracer. Hands/wrists were more commonly contaminated than the head/face (57% vs. 23% of swabs with PSL detection, respectively). One subject had PSLs detected by the breathing zone air sampler with high concentration (9.7×10^5 PSL/L air). Future work will further investigate this potential inhalational risk. Overall, this study provides a well-characterized method that can be used to quantitate levels of skin and inhalational contact with simulant pathogen particles. The PSL method serves as a complement to the fluorescent tracer method to study PPE doffing self-contamination.

2HA.21**PM_{2.5} Generated during Rapid Failure of Fiber-reinforced Concrete Induces TNF-alpha Response in Macrophages.**

LUPITA MONTOYA, Harish Gadde, Wyatt Champion, Ning Li, Mija Hubler, *University of Colorado Boulder*

Failure of large, concrete structures can lead to the generation of very small fragments, including aerosols in the fine fraction, which have aerodynamic diameters of ≤ 2.5 micrometers (PM_{2.5}). These aerosols can persist in the environment, pose exposure risks, and potentially cause negative health effects. New trends in construction favor the use of concrete reinforced with steel fibers, but little is known about the nature of the fragments generated during its failure. This study investigated the fragmentation of several steel-fiber reinforced concrete formulations using dynamic compression testing. The release of tumor necrosis factor alpha (TNF- α), an inflammatory marker widely used in both human and animal studies, was then analyzed to determine the effects of the fragments in the aerosol fine fraction on mouse macrophages (RAW 264.7). All concrete formulations studied showed statistically increased TNF- α release, which was inversely correlated with fiber length and fiber content (%weight). In addition, results from a select set of concrete formulations also showed a clear dose-response relationship. This paper postulates the fracture mechanisms by which concrete parameters (i.e., fiber length and content) lead to the generation of PM_{2.5}, producing the observed TNF- α release.

2IM.1**Traffic Related Aerosols Measurement with HR-ELPI+ Using Sintered Collection Plates.** ANSSI ARFFMAN, Peter Lambaerts, Markus Nikka, Erkki Lamminen, *Dekati Ltd.*

In this study, the performance of HR-ELPI+ (Dekati Ltd.) inversion with sintered collection plates on soot and urban aerosols were investigated. The HR-ELPI+ was challenged with diesel soot and traffic emitted aerosols, and the experimental results were analysed using numerical methods. Elaborate analysis of the results was performed as the calibration of instrument is provided only for the spherical liquid aerosols. This needs to be understood, when comparing measurement results between instruments based on the different physical measurement principles.

Soot aerosol for the experiments was generated with idling diesel passenger car. The exhaust gas was first diluted with the eDiluter (Dekati Ltd.) using heated primary dilution to avoid the condensation of volatile gas phase species on soot (200°C). After the dilution, the exhaust particle size distribution was measured with two HR-ELPI+'s equipped with plain and sintered collection plates, and an SMPS (model 3082, TSI Inc.) Measurement results were further analyzed by numerically simulating the instrument response for different primary particle size and mass fractal dimensions, and their effect on the HR-ELPI+ inversion were quantified. Long-term urban aerosol measurements were conducted at the air quality measurement station in Finnish inland city, and the time series results were analysed in the study.

Results of the study showed that the HR-ELPI+ with sintered and plain collection plates provides consistent results for agglomerated soot particles. The inversion was found to behave similarly with the normal ELPI+ calculation (cut-point concept) with respect to the effective density value that is a robust feature regarding the inversion. Results also showed that the average aerodynamic particle size was below the average mobility particle size in all measurements giving the average effective density below the unit density value.

2IM.2

Instrument Artifacts Lead to Uncertainties in Parameterizations of Cloud Condensation Nucleation. JESSICA MIRRIELEES, Sarah Brooks, *Texas A&M University*

The concentrations of cloud condensation nuclei (CCN) modulate cloud properties, rainfall location and intensity, and climate forcings. This work assesses uncertainties in CCN measurements and the apparent hygroscopicity parameter (κ_{app}) which is widely used to represent CCN populations in climate models. CCN measurements require accurate operation of three instruments: the CCN instrument, the differential mobility analyzer (DMA), and the condensation particle counter (CPC). Assessment of DMA operation showed that varying the ratio of aerosol to sheath flow from 0.05 to 0.30 resulted in discrepancies between the κ_{app} values calculated from CCN measurements and the literature value. Discrepancies were found to increase from < 1% to 13% for both sodium chloride and ammonium sulfate. The ratio of excess to sheath flow was also varied, which shifted the downstream aerosol distribution towards smaller particle diameters (for excess flow < sheath flow) or larger particle diameters (for excess flow > sheath flow) than predicted. For the CPC instrument, undercounting occurred at high concentrations, resulting in calculated κ_{app} lower than the literature values. Lastly, undercounting by CCN instruments at high concentration was also assessed, taking the effect of supersaturation on counting efficiency into account. Under recommended operating conditions, the combined DMA, CPC, and CCN uncertainties in κ_{app} are 1.2 % or less for 25 to 200 nm diameter aerosols.

2IM.3

Improved Coincidence Correction in Condensational Particle Counters. STEVEN SPIELMAN, Gregory Lewis, Susanne Hering, *Aerosol Dynamics Inc.*

As with any instrument that records discrete events, an airborne particle counter can benefit by correcting for the fact that multiple particles can arrive simultaneously. For this work, we assume that condensationally-enlarged particles scatter light, which is captured by an optical detector and converted into an electrical signal. Pulse heights in this application are fairly uniform, even though the average rate can vary by many orders of magnitude. At low concentration, particles can be accurately counted by simply triggering on every pulse that exceeds some threshold. However, while the signal is above the threshold, the detector cannot detect an additional particle. This "dead time" can be inferred by assuming fixed pulse width, or by direct measurement. Some instruments, for example the TSI 3787, further refine the correction by recognizing that nearby pulses tend to join, due to the overlap of their tails. This technique works well up to an average particle rate of about 1.0 particles per FWHM (the full-width at half-maximum of a pulse) with a measured dead time of 80%. It fails at higher concentrations, when pulses are likely to include three or more particles.

We have developed a coincidence correction algorithm that can handle average pulse rates as high as 3.0 particles per FWHM. Accurate particle concentrations can be determined even with a dead time of 99.5%. We present modeling and experimental results, with both AC- and DC-coupled systems.

2IM.5**The Caltech nano-Scanning Electrical Mobility Spectrometer (nSEMS): Design, Modeling, and Characterization for Size Distribution Measurements in the Low Nanometer Regime.**

STAVROS AMANATIDIS, Weimeng Kong, Huajun Mai, Yuanlong Huang, Richard Flagan, *The CLOUD Collaboration, California Institute of Technology*

We present the design, modeling and experimental characterization of the Caltech nano-Scanning Electrical Mobility Spectrometer (nSEMS), a recently developed instrument designed to probe particle formation and growth at the "CLOUD" experiment at CERN, Switzerland.

The nSEMS consists of a charge conditioner, a novel differential mobility analyzer, and a two-stage Condensation Particle Counter (CPC). The mobility analyzer was designed and optimized for size classification in the 1.5 – 25 nm range with minimal diffusional losses through 3D finite element modeling of the flows, electric field, and particle trajectories. The classifier operates on a dual high-voltage supply with fast polarity-switching capability to minimize sensitivity to variations in the chemical nature of the ions used to charge the aerosol.

The nSEMS employs a new soft x-ray charge-conditioner that was designed to optimize both particle charging and transmission efficiency in the low nanometer regime. The CLOUD experiment, for which this instrument was designed, probes neutral nucleation by removing all ions from the chamber, and nucleation of clusters on ions produced by galactic cosmic rays, or by a pion beam to probe particle formation under upper-tropospheric conditions. With the soft x-ray source turned on, the nSEMS can, therefore, probe neutral-cluster nucleation; with it turned off, it can measure particles formed by ion-induced nucleation. Particles transmitted through the charge-conditioner and mobility analyzer are measured using a two-stage CPC. The particles are first activated in a fast-mixing diethylene glycol stage that was developed at Caltech; the second, booster and detection stage, is a TSI Model 3760A, butanol CPC.

We will describe the design of the various components of the instrument, and the experimental characterization of the individual components, charge conditioner, mobility classifier, and two-stage CPC, present the transfer function of the integrated instrument, and examine its measurements of transient nucleation and growth events in the CLOUD chamber.

2IM.6**Development of a Respirable Virtual-Cyclone Sampler.** HONG-YANG CHEN, Chih-Wei Lin, Ting-Ju Chen, Sheng-Hsiu Huang, Yu-Mei Kuo, Chih-Chieh Chen, *National Taiwan University*

Health-based aerosol sampling should reflect how particles penetrate and deposit in the various regions of the human respiratory system. Therefore, size-selective sampling should be adopted when monitor aerosol concentration in the atmosphere. However, most samplers can only match the 50% cut point, but not the slope defined by the international community. Additionally, cyclone samplers were found to be affected by the aerosol deposition on the wall of the cyclone body, which leads to a significant decrease in aerosol penetration. A virtual cyclone was used to overcome the loading effect, but still had the disadvantage of showing high aerosol penetration on the large particle size. In this work, the configurations of the virtual cyclones were further studied to eliminate the tailing phenomenon of the separation efficiency curve. The new virtual cyclones successfully demonstrate accurate and constant measurement of the atmospheric dust component, and thus the extent of health hazards.

2IM.8

A New Aerosol Dynamics Scanning WCPC. GREGORY LEWIS, Arantzazu Eiguren Fernandez, Steven Spielman, Susanne Hering, *Aerosol Dynamics Inc.*

Aerosol size distributions are typically measured using a DMA and particle counter. Mobile applications and those evaluating changing aerosols require fast particle counters for measuring particle size distributions. Due to charging inefficiencies only a small percentage of particles are detected, especially for particles in the 1 to 10 nm range.

Aerosol Dynamics has developed a new water condensational particle counter that can scan temperatures, varying the 50% activation efficiency from below 2nm to 7nm. This eliminates the need for a charger and DMA. A up scan can be completed in as little as one minute. We present data from the 2019 Helsinki CPC Workshop and subsequent lab and field tests.

The new instrument uses a “pseudo sheath”, in which the outer slower moving portion of the aerosol flow is removed after the first cold section (i.e. the conditioner). Unlike true sheathed instruments, the aerosol flow is directly measured rather than calculated by the difference between total flow and the sheath flow. We also explored changes in flow rates, lengths of the three sections of the growth tube and bore diameter.

These design changes produce a fast response time and sharper cut-off, which improves size distribution measurements with traditional DMAs. Preliminary results indicate a 3-tau (5% to 95%) of about 200ms, and further optimization may reduce this further.

2IM.9

Laboratory Evaluation of an Engine Exhaust Particle Sizer (EEPS) Spectrometer for Fast Measurements of Particle Number Size Distributions in Aircraft Exhaust Plumes. YOSHIKO MURASHIMA, Hiromu Sakurai, Yuji Fujitani, Nobuyuki Takegawa, *AIST*

We used a TSI Engine Exhaust Particle Sizer (EEPS) spectrometer (model 3090) to measure particle number size distributions in aircraft exhaust plumes during a field experiment at the Narita international airport. The accuracy of particle sizing and concentration measurement in the size range relevant to aircraft exhaust nanoparticles (~6-100 nm) are critical for interpreting the field data. We have set up apparatuses for evaluating the EEPS with monodisperse and polydisperse aerosols using a reference condensation particle counter (CPC) and scanning mobility particle sizer (SMPS) spectrometer that can be traced to particle standards maintained by the National Institute of Advanced Industrial Science and Technology. Test aerosol particles (either polydisperse or monodisperse) were measured in parallel with the EEPS, the reference CPC, and the reference SMPS. The total number concentration that was obtained by integrating the size distribution measured by the EEPS was compared with the number concentration measured by the reference CPC. The size distribution function ($dN/d\log d$) at each size bin was compared between the EEPS and the reference SMPS. We used polydisperse silver particles with the modal diameter of ~10 nm by evaporation/condensation generator, and mobility-classified monodisperse polystyrene latex particles at 30, 60, 100, and 200 nm. We have found that the EEPS tends to underestimate the number concentration in the size range from 6 to 30 nm.

2IM.11

Development of an Aerosol Concentrator/Diffusion Battery Tandem for Evaluating the Toxicological Properties of Concentrated Ambient Accumulation Mode Particles in Controlled Inhalation (In-vivo) Exposure Studies. MILAD PIRHADI, Amirhosein Mousavi, Sina Taghvaei, Mohammad Sowlat, Constantinos Sioutas, *University of Southern California*

The ability to conduct exposures using the concentrated ambient accumulation mode particles separately from ultrafine particles (UFPs) has been a serious challenge in the health studies. In this study, we were able to overcome this major limitation in exposure studies by designing and evaluating the performance of a tandem technology, consisting of the developed versatile aerosol concentration enrichment system (VACES) and a screen-type diffusion battery, which removes ambient UFPs from the airflow, enabling us to directly conduct exposure studies on concentrated ambient accumulation mode particles (0.18-2.5 μm). First, we evaluated the performance of the diffusion battery using various types of laboratory-generated aerosols under controlled conditions. The optimum operational flow rate (5 lpm) and number of stages (6 stages) of the diffusion battery was selected based on the lab tests. We subsequently deployed the diffusion battery in our sampling site in the Los Angeles, and connected it to the VACES in order to evaluate the VACES/diffusion battery performance using the ambient fine particulate matter (PM_{2.5}). The field tests results confirmed the capability of the tandem technology to concentrate efficiently the ambient accumulation mode PM while the majority of the UFPs are removed from the concentrated aerosol. The diffusion battery illustrated a 50% cut-point of around 100 nm, and the removal efficiency of particles less than 50 nm exceeded 70–90%. The mass concentrations and chemical composition of the ambient accumulation mode particles collected using the tandem technology compared with those collected with a reference sampler, MOUDI, in parallel vary around 5-15%. This excellent agreement further corroborates the high efficiency of the VACES/diffusion battery tandem technology to directly conduct exposure studies on concentrated ambient accumulation mode PM.

2IM.12

Light Absorption by Ammonium Sulfate with Carbon Black Inclusions: Experiments, Mie Theory and Effective Medium Approximations. JAMES RADNEY, Christopher Zangmeister, *National Institute of Standards and Technology*

The refractive index of aerosols is one of the key parameters in determining the optical properties, and hence the radiative forcing, with Mie theory being the calculation method of choice due to its ease of use and computational efficiency. Typically, for complex multi-component aerosols, e.g. biomass burning aerosols with black carbon inclusions, only an effective refractive index corresponding to a specific fuel type or specific burn can be retrieved from measurements. Here, we measure the extinction and absorption cross-sections of size- and mass-selected particles composed of non-absorbing ammonium sulfate with strongly absorbing carbon black inclusions at multiple mass fractions. We then compare refractive indices retrieved using Mie theory assuming: 1) homogeneous particles, 2) a core-shell configuration and 3) a variety of effective medium approximations (e.g. volume mixing, Maxwell-Garnett, Bruggman, etc.) to those obtained from spectroscopic ellipsometry utilizing the same mixtures. The goal of this work is to determine if consistent refractive indices for the two materials (ammonium sulfate and carbon black) across the multiple mass fractions can be obtained from these approximations thereby validating these simplistic computational approaches to a complex modeling problem.

2IM.13

Assessing Respirator Protection Factor with Novel Personal Devices. MARGARET SIETSEMA, Thomas Peters, Allison Persing, K.R. Farmer, *University of Iowa*

Background: Respirators are worn by medical professionals, emergency responders, construction workers and industrial workers to reduce their inhalation exposure to aerosols. A fit test is performed when a respirator is initially assigned to a worker and annually thereafter to assess the protection the respirator provides. Quantitative fit testing is typically conducted using the TSI PortaCount[®], a single-channel bench-top device that uses an alcohol-based condensation particle counting system to measure the particle concentration inside and outside of the respirator.

Aim: To evaluate two new, compact (<0.8 kg, <950 cm³) and wearable dual channel particle counters that would enable real-time respirator fit evaluation. One instrument uses a dual channel optical particle counter (DC-OPC) while the other uses a dual channel water-based CPC (DC-CPC) to measure particle concentrations simultaneously inside and outside the respirator facepiece.

Methods: Respirator fit factors measured simultaneously from a PortaCount[®] (real-time mode), the DC-OPC, and the DC-CPC were compared for one test subject for three aerosols (ambient, sodium chloride, and smoke) over a range of protection factors and aerosol concentrations. The experiments were run using a 3M 65021HA1-C Household Multi-Purpose Respirator with P100 organic vapor cartridges. During testing, three OSHA accepted activities for determining a fit factor were performed, including normal breathing, deep breathing, and moving the head side to side.

Results: The DC-CPC correlates well with the PortaCount[®] over a wide range of protection factors up to at least 2000, ambient aerosol concentrations and aerosol types. Second-by-second protection factor variations due to breathing or other changes in the subject's activity are captured by the DC-CPC and correlate well ($R^2 > 0.8$) with fluctuations measured by the PortaCount[®]. In contrast, the DC-OPC has a limited functional range in ambient concentrations between ~10,000 and ~40,000 p/cm³ and for protection factors less than ~100.

2IM.14

Development of an Innovative Aerosol Generation Setup for In-vivo Exposure Studies. SINA TAGHVAEE, Amirhosein Mousavi, Mohammad Sowlat, Constantinos Sioutas, *University of Southern California*

In this study, we developed a new setup for generating particles that perfectly resemble ambient particulate matters (PM) in terms of physical and chemical properties. The ambient PM samples were collected on filters using a high volume sampler; followed by their extraction in Milli-Q water. In an alternative approach, we captured the ambient PM samples directly into Milli-Q water using the versatile aerosol concentration enrichment system (VACES)/aerosol-into-liquid collector tandem technology. Commercial HOPE nebulizers were then implemented for re-aerosolizing aqueous PM slurries from these two approaches. To assess the physical properties of generated particles, their size distributions were investigated at different compressed air pressure of the nebulizer, and dilution flow rate by the means of a scanning mobility particle sizer (SMPS) in conjunction with a condensation particle counter (CPC). Moreover, chemical analysis were conducted on ambient, and re-aerosolized samples to determine their chemical components including elemental and organic carbon (EC/OC), water soluble organic carbon (WSOC), polycyclic aromatic hydrocarbons (PAHs), metals and trace elements, and inorganic ions. Our finding revealed that re-aerosolizing the aqueous extracted PM slurries will provide us with effective recovery of the water soluble constituents of ambient PM including water soluble organic matter, and water soluble inorganic ions. However, this approach is unable to recover water insoluble constituents of ambient PM such as EC, PAHs, and some of the redox-active metal elements. Conversely, re-aerosolizing the directly captured PM slurry collected via the means of VACES/aerosol-into-liquid collector tandem technology was able to perfectly reconstruct all constituents of ambient PM. Therefore, our results underscore the advantages of VACES/aerosol-into liquid collector tandem technology to collect aqueous slurries of ambient PM; followed by their re-aerosolization to generate stable aerosols that are well representative of ambient PM.

2IM.15

Development of an EHD Induced Wind Driven Personal Exposure Monitor and In-situ Analysis for Characterization of Exposure. RAVI SANKAR VADDI, Gaurav Mahamuni, Igor Novosselov, *University of Washington*

Exposure to ultrafine particulate matter (UPM) from combustion and manufacturing processes can cause adverse health effects. The toxic potential of inhaled particles depends on particle size and their chemical composition. Collection of air-borne particles on a filter and their chemical analysis is costly and time-consuming. We demonstrate a novel ultrafine particle electrostatic collector that uses a corona wire to rod discharge that provides the electrohydrodynamic (EHD) driven flow for particle aspiration and for charging the particles. The particles are then directed on to a quartz slide coated with polydimethylsiloxane (PDMS) due to the electric field between the collection and repelling electrodes. Collection of particles on an optically transparent substrate is advantageous and enabling an in-situ analysis of collected UPM. The sensor prototype has been tested using the combustion-generated UPM, i.e., cigarette smoke, diesel exhaust, wood smoke, and ethane soot from laboratory inverted gravity flame reactor (IGFR) operated at two different temperatures. Upon collection of the UPM sample, the PDMS acts as a solid phase extraction media for polyaromatic hydrocarbon (PAH) associated with UPM. Excitation-Emission Matrix (EEM) fluorescent spectroscopy is used to characterize the PAH content of the UPM. We compare EEMs for the samples collected (i) on the filter followed by liquid extraction into cyclohexane and (ii) collection on a transparent substrate with subsequent in-situ solid phase extraction into PDMS. The latter method compares well with the liquid extraction method and can potentially be used as a compact, low-cost sensor.

2IM.16

Retrieval of High Time Resolution Growth Factor Probability Density Function from a Humidity-controlled Fast Integrated Mobility Spectrometer. YANG WANG, Guangjie Zheng, Steven Spielman, Tamara Pinterich, Susanne Hering, Jian Wang, *Washington University in St. Louis*

Hygroscopicity describes the tendency of aerosol particle to uptake water and is among the key parameters in determining the impact of atmospheric aerosols on global radiation and climate. A hygroscopicity tandem differential mobility analyzer (HTDMA) system is the most widely used instrument for determining the aerosol hygroscopic growth. Because of the time needed to scan the classifying voltage of the DMA, HTDMA measurement often requires a minimum of 30 min to characterize the particle hygroscopic growth at a single relative humidity for 5 to 6 different sizes. This slow speed is often inadequate for measurements onboard mobile platforms or when aerosols evolve rapidly. Recently, a humidity-controlled fast integrated mobility spectrometer (HFIMS) was developed for measuring the hygroscopic growth of particles. The measurement speed of the HFIMS is about one order of magnitude faster than that of the conventional HTDMA.

In this work, a data inversion routine is developed to retrieve the growth factor probability density function (GF-PDF) of particles measured by the HFIMS. The inversion routine considers the transfer functions of the upstream DMA and the downstream water-based fast integrated mobility spectrometer (FIMS), and derives the GF-PDF that reproduces the measured responses of the HFIMS. The performance of the inversion routine is examined using ambient measurements with different assumptions for the spectral shape of the particle GF-PDF (multimodal lognormal or piecewise linear). The influences of the data inversion parameters and counting statistics on the inverted GF-PDFs were further investigated, and an approach to determine the optimized inversion parameters is presented.

2IM.17**Thermal Decomposition Characterization of Filter Inlet for Gases and AEROSols (FIGAERO) Coupled with Chemical Ionization Time-of-Flight Mass Spectrometer (ToF-CIMS).**

LAURA YANG, Masayuki Takeuchi, Nga Lee Ng, *Georgia Institute of Technology*

There have been several studies on the effects of thermal decomposition on the interpretation of FIGAERO data, but no systematic study has been conducted to fully characterize the thermal decomposition behaviors nor the impact of instrument parameters on thermal decomposition. The objectives of this project are 1) to evaluate the mechanisms of thermal decomposition (i.e., decarboxylation and dehydration) in the FIGAERO using a suite of standard compounds with carboxylic acid and/or alcohol groups, and 2) to provide qualitative and quantitative means to infer the degree of thermal decomposition in the FIGAERO data by identifying patterns in measurement parameters, such as decomposition temperature and time profile. The temperature ramping rate effect is investigated as sub-objectives. Standard compounds of choice for testing include 1,2,3,4-butanetetracarboxylic acid, di-pentaerythritol, and citric acid. Each standard compound was diluted to 0.1 g/L and thermally desorbed at a temperature rate of 10 C/min, soaked for 20 minutes, and cooled for 10 minutes. Furthermore, experiments were conducted with different temperature ramping rates: < 15 min (fast), 15 minutes (normal), and > 15 minutes (slow) with citric acid while maintaining the soaking and cooling times constant. For 1,2,3,4-butanetetracarboxylic acid and citric acid, dehydration is observed to be the major thermal decomposition behavior with each dehydrated product desorption signal peak appearing sequentially (i.e., 1,2,3,4-butanetetracarboxylic acid desorption temperature: C₈H₁₀O₈: 155C, C₈H₈O₇: 165C, and C₈H₆O₆: 170C). Moreover, the thermal desorption profile of normal ramping rate exhibits a distinctive pattern from that of the other ramping rates. This could be due to chemical compound behaving differently under a varying temperature gradient. This study provides new insights into how to choose the best instrumental parameters to obtain consistent results when using FIGAERO for aerosol studies.

2IM.18**Effects of Fluorescence Removal on the Raman Spectra of Single Atmospheric Aerosol Particles.** DAVID DOUGHTY, Steven Hill, *CCDC Army Research Laboratory*

Raman spectroscopy can be used to provide information on the chemical composition of individual aerosol particles. Fluorescence can interfere with analysis of Raman spectra, and in some cases can completely obscure the Raman signal. Estimating and removing fluorescence from Raman spectra is a commonly used analysis technique. We show that for spectra with D/G Raman peaks, the individual-particle fluorescence spectra can vary greatly. These variations suggest differing fluorescent materials associated with different particles. We also illustrate the effects of different fluorescence removal algorithms on the peak locations of the D and G bands. The use of both fluorescence and Raman spectra may be especially helpful in individual particle analysis, where the particles are small (e.g., 200 nm) and the goals include measuring sufficient number of spectra to obtain time variations and useful statistics for ambient particles. That is, analysis of both fluorescence and Raman spectra may help in identifying more types of atmospheric particles.

2IM.19

Measurement of Aircraft Engine Soot Emissions using the ESCOM – the Engine Soot Compliance Monitor. ANDREW FREEDMAN, Zhenhong Yu, Richard Miake-Lye, Timothy Onasch, *Aerodyne Research, Inc.*

The International Civil Aviation Organization (ICAO) has set emissions standards for non-volatile PM (nvPM) emissions, primarily light absorbing carbon, from aircraft engines. It relies on the SAE E-31 Committee to draw up specific technical standards for the measurement of these emissions as well as certification procedures for nvPM emission monitors. Currently, two instruments have been certified with the committee's criteria. In order to meet the need for another measurement approach, Aerodyne Research is developing the Engine Soot Compliance Monitor (ESCOM) based on its CAPS PM_{SSA} monitor.

The ESCOM monitor, operating on CAPS technology, provides an accurate mass-based measurement of nvPM emissions from aircraft engines that can meet the requirements for ICAO-based compliance testing. In addition to measuring the mass-based emissions, the ESCOM provides a real-time measure of the emission index and single scattering albedo (SSA). The Aerodyne ESCOM monitor was characterized in the laboratory using flame soot and participated in the EPA sponsored VARIAnT2-4 studies and NASA sponsored ND-MAX campaign. Results will be shown from these field tests, which involved sampling from in-use, on-wing engines and engines on test stands burning various types of biofuel mixtures as well as standard jet fuel.

2IM.20

Theoretical and Experimental Analysis of the Core Sampling Method: Reducing Diffusional Losses in Aerosol Sampling Line. Yueyun Fu, Mo Xue, Runlong Cai, Juha Kangasluoma, JINGKUN JIANG, *Tsinghua University*

Core sampling method (extracting a portion of a flow from the core of the flow) will reduce diffusional losses of highly diffusive species (e.g., aerosol nanoparticles, ions, and gases) when transporting them through a sampling tube. Revealing parameters governing the sampling efficiency of a core sampling system, η_{sam} , helps to design the apparatus and to optimize its performance. In this study, we report an analytical solution for quantifying the η_{sam} by solving the convection diffusion equation of laminar flow field. The analytical results were experimentally evaluated using 1-5 nm tungsten oxide nanoparticles. η_{sam} is governed by a dimensionless loss parameter and the transport-to-sample flow ratio.

Theoretically predicted values for η_{sam} agree with experimental results, e.g., the relative deviation is within 5% when the value for the loss parameter is less than 0.1. The core sampling method is recommended to work at the loss parameter less than 0.1 such that η_{sam} is equal or close to the maximum value of unity and is also insensitive to variations in sampling conditions. How to apply the findings in designing and optimizing a core sampling system was discussed. A core sampling apparatus was then designed and experimentally evaluated. Its sampling efficiency was shown to be significantly higher than those of a tee, a cross fitting, and a Y fitting when the same sampling conditions were used.

Fu et al., 2019, *Aerosol Science and Technology*, in press (online available: <https://doi.org/10.1080/02786826.2019.1608354>)

2IM.22**The Transfer Function of a Drift Tube Ion Mobility Spectrometer-Condensation Particle Counter Combination.**

JIHYEON LEE, David Buckley, Jikku Thomas, Christopher Hogan Jr., *University of Minnesota*

Our laboratory group has developed an atmospheric pressure drift tube ion mobility spectrometer (DTIMS), which can be coupled to a condensation particle counter (CPC). The DTIMS-CPC combination enables rapid (< 20 seconds) and adaptable size distribution measurements up to ~40 nm in size, with an optimum size range of 4-30 nm. To classify particles the DTIMS utilizes the same particle property as the differential mobility analyzer, i.e. electrical mobility, but instead of spatially filtering particles, it temporally separates them in a linear electric field, such that their arrival time at the CPC detector is inversely proportional to the electrical mobility. The transfer function of the DTIMS is necessary to convert the concentration per arrival time to concentration per unit mobility or to size distribution function. We have determined the transfer function for the most recent version of the DTIMS-CPC system (Kanomax FMT Model 3006), which operates with 10 kV applied across the DTIMS inlet and is coupled with a subsecond response CPC. A Twomey-Markowski algorithm was used to derive the transfer function from differential mobility analyzer-DTIMS-CPC measurements. For the verification of the transfer function, sodium chloride particles generated by a nano-aerosol generator (NAG) were measured by the DTIMS-CPC and the inverted mobility distributions were compared to the results from a commercially available differential mobility analyzer. The comparison results show that the transfer function of DTIMS for particles up to 40 nm is successfully determined to imply the wider application of the device.

2IM.23**Comparison between Dimethyl phthalate and Diethylene glycol as a Working Fluid of a Laminar Flow Particle Size Magnifier.**

KENJIRO IIDA, Hiromu Sakurai, Tetsuji Koyama, Tsuyoshi Taishi, *AIST*

A laminar flow particle size magnifier (PSM) was developed and coupled to a condensation particle counter (CPC) to detect aerosol particles in less than 10 nm particle diameter range. The performance of the PSM-CPC system (called "the system") was evaluated using a diethylene glycol (DEG) and dimethyl phthalate (DMP). False counts rates induced by homogeneous nucleation of working fluid (WF) vapor were evaluated as a function of saturator temperature. The false count rate (FCR) of DEG based system is significantly affected by water-vapor in a sample flow indicating that binary homogeneous nucleation between DEG and water vapor induces false counts. Whereas FCR of DMP-based system is minimally affected by water vapor in a sample flow indicating that false counts remain stable regardless of the variation in the relative humidity of sampled aerosol. Detection efficiencies of the system were evaluated using negatively charged NaCl and Ag aerosol over 1.0 to 10 nm particle diameter range. The efficiency curve of DEG-based system had higher plateau value (=0.93) than DMP-based system did (=0.84). The value of d_{50} , which is the particle diameter at 50% detection efficiency, showed that d_{50} of DMP-based system are less dependent on particle material than DEG-based system are. DEG-based system detects less than 1 nm NaCl particles, and the observed trend is most likely related to that bulk NaCl crystals dissolves in DEG liquid.

2IM.24

PM2.5 Concentration Prediction Using Convolutional Long Short-Term Neural Network. KAZUSHI INOUE, Ayumi Iwata, Tomoaki Okuda, *Keio University*

Environmental standard for PM2.5 concentration is provided as a standard value for achieving appropriate protection of human health. Apart from this, there is a provisional guideline as an alerting when it is predicted that the concentration of PM2.5 will be too high. However, existing prediction methods for PM2.5 concentration are often inaccurate over a long period, such as 12 hours ahead, and have not been able to play an effective role in decision making for alerting. Therefore, we tried to predict PM2.5 concentration after 12 hours using deep neural network. We proposed the method of combining the convolutional neural network (CNN) and the long short-term memory (LSTM) to extract the spatiotemporal relationship of the PM2.5 concentration. CNN is a method widely used mainly in the field of image processing, and it is possible to extract image features. In this study, we mapped the concentration data at each air quality monitoring station, reflecting its positional relationship, to generate "PM2.5 concentration image". The spatial relationship between adjacent monitoring stations was extracted by using the CNN method on this image. After extracting the spatial relationship in this method, it was combined with the LSTM. LSTM is a method for handling time series data, and it is possible to extract temporal relationships. Spatiotemporal features at arbitrary points were extracted by inputting time-series data of spatial relationships extracted by CNN into LSTM. These proposed spatiotemporal features were combined with auxiliary data such as date and time, and meteorological data such as wind speed and temperature to generate the proposed model and to predict PM2.5 concentration. In addition, the datasets used to verify the effectiveness of the proposed model were all obtained from Atmospheric Environmental Regional Observation System: AEROS.

2IM.25

Accelerated Size Distribution Measurements using a Scanning Aerodynamic Aerosol Classifier. TYLER J. JOHNSON, Jonathan Symonds, Jason S. Olfert, Adam M Boies, *University of Cambridge*

The Aerodynamic Aerosol Classifier (AAC) selects particles based on their relaxation time by passing the aerosol between spinning concentric cylinders with a sheath flow. Johnson et al. (2018) demonstrated that the aerodynamic size distribution of the aerosol is measured by stepping the AAC setpoint and quantifying the classified particle number concentration at each steady-state condition. However, this approach is similar to stepping a Differential Mobility Analyzer (DMA) in a Differential Mobility Particle Sizer (DMPS) system. In either sizing system, the stepping procedure requires long times to achieve sufficient size spectral resolutions. This limitation was overcome in the DMPS by Wang and Flagan (1990) developing the Scanning Mobility Particle Sizer (SMPS).

This study follows a similar methodology and demonstrates size distribution measurements are accelerated by continuously changing rather than stepping the AAC classifier speed. By varying the speed following an exponential function, the change in centrifugal force a particle experiences during its classifier residence time is independent of its inlet time, and the scanning AAC transfer function converges to the same shape as produced during steady-state operation. The high agreement between aerodynamic size distributions of three different aerosol sources (DOS, salt and soot) independently measured by stepping and scanning the AAC validates this new methodology. For instance, the Count Median Diameter (CMD), Geometric Standard Deviation (GSD) and total number concentration of the DOS size distribution measured by the stepping and scanning AAC agreed within 0.55%, 0.12% and 1.05% at low flow, respectively.

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2IM.26

Improvement of Cyclone Sampler and Its Performance for Chemical Composition and Toxicity Measurement. TAKUYA KATORI, Ayumi Iwata, Daiki Shishido, Yoshihiro Terui, Tomoaki Okuda, *Keio University*

In order to evaluate the adverse human effect of PM_{2.5}, generally, these particles have been collected on a filter. However, this method is potentially unsuitable for toxicity evaluation of the particles. The reasons for that are as follows: (1) some previous studies have reported that the collected volatile components are evaporated from the filter during sampling periods (negative artifact), and (2) particles collected and entangled in the filter fibers are difficult to be removed and thus it is difficult to conduct the biological exposure experiments. Therefore, filter method is not suited for toxicity evaluation of the particles. Our previous work developed a high volume cyclone sampler to overcome these above problems. As a result, we could collect a large amount of atmospheric particles as powder form, thus we could conduct these exposure experiments. However, we did not conduct the detailed performance evaluation of our sampler. We further improved this cyclone sampler, and demonstrated that the new sampler is more suitable for measuring the chemical compositions and toxicities of the particles. According to the separation performance measurement for the previous cyclone sampler using monodisperse fluorescent particles, this sampler was found not to collect smaller particles than 0.7 μm at 1,200 LPM. In order to solve these problems, we improved by using a smaller cyclone. The separation performance measurements with this improved cyclone method indicated that the larger atmospheric particles than approximately 0.14 μm at 125 LPM could be collected. Furthermore, the comparison of chemical composition measurement in filter sample and cyclone sample revealed that the cyclone method significantly prevents the negative artifact than the filter method. Therefore, this new cyclone sampler was improved to solve the potential problems with filter sampling and previous cyclone sampling. We will also show the toxicity analysis result of the particles collected with this cyclone.

2IM.27

Comprehensive Detection of All Analytes in a Large Chromatographic Dataset of Complex Environmental Samples. SUNGWOO KIM, Gabriel Isaacman-VanWertz, *Virginia Polytechnic Institute and State University*

Gas chromatography/mass spectrometry is a common analytical method used in environmental analysis to separate and identify individual compounds within a complex mixture. However, in nearly all cases, data reduction requires manual inspection of representative chromatograms to catalog potential chromatographic peaks of interest for more in-depth analysis. This approach represents unique challenges in the analysis of complex environmental mixtures. Ambient aerosols may contain hundreds or thousands of unique organic compounds, and even minor components may provide valuable insight into particle sources and formation chemistry. Furthermore, due to the highly dynamic nature of aerosol composition so many chromatograms may need to be inspected to fully catalog all constituents. These difficulties have limited comprehensive chromatographic analysis of atmospheric aerosols, with typically only a few dozen analytes reported for a dataset and the discarding of a large amount of potentially useful data. We present here an automated approach of cataloging and potentially identifying all analytes in a large chromatographic dataset of ambient aerosols. We use Positive Matrix Factorization (PMF) of small sub-sections of multiple chromatograms to extract factors that describe individual or small numbers of analytes. Potential chromatographic peaks in these factors are evaluated based on features such as peak shape, noise, and retention time. With our approach, all analytes within the small section of the chromatogram are cataloged, and the process is repeated for overlapping sections across the chromatogram, generating a complete list of the retention times and estimated mass spectra of all peaks in a dataset. As a case study, we demonstrate that in real-world chromatograms of ambient aerosols, even a small (e.g. 10 second) section of a chromatogram may contain several dozen chromatographic peaks. We demonstrate that this method extracts peaks that appear in only a fraction of chromatograms, so provides an automated and means to build a complete list of analytes in a dataset with minimal user interaction.

2IM.28

An Aerosol Particle Monitor for Use in Micro-Gravity Cabin Exposure Studies. NATHAN KREISBERG, Steven Spielman, Gregory Lewis, Susanne Hering, Tim Gordon, Gavin McMeeking, *Aerosol Dynamics Inc*

Given the majority of personal exposure to airborne particulates occurs indoors, instrumental methods are needed tailored to different indoor environments. One novel environment is micro-gravity aerospace cabins such as the International Space Station (ISS) that impose operational constraints and significant limits on size, power, and permissible materials. Despite active filtration measures in place, little is known about potential human exposure to particulates including concentration and size. The absence of gravitational settling greatly extends the range of interest for particle size. A real-time monitor is needed to correlate human activity believed to be the primary source of particle generation. Here we describe the adaptation of two traditional particle measurement technologies, condensation particle counting and light scattering particle sizing, into an aerosol particle monitor (APM) for use on the ISS.

In a compact, integrated package the APM incorporates a modified water condensation particle counter (WCPC) and a modified commercially available portable optical particle spectrometer (POPS). To avoid water handling or use of a reservoir, a water recycling system was developed for the WCPC enabling startup from a dry state (i.e. liquid-free launch) by harvesting moisture from the cabin. A virtual impactor stage, designed using numerical modeling, was built into the inlet to compensate for the low flow of the spectrometer while coupling them was facilitated through conversion of the POPS to use a re-circulating sheath flow. Additionally, the size range of the POS was modified to extend particle sizing from the original 0.2-3 μm to 1-10 μm to complement the fine aerosol concentration measured by the WCPC. This shift in range is fully reversible so that the original POPS size range can be easily recovered. The benefits of long term, unattended operation of the APM design extend to other environments needing real-time, continuous particle monitoring.

2IM.29

Elucidation of Electrostatic Charging Characteristics of Radioactive Cs-Bearing Particles by Kelvin Probe Force Microscopy. KEIICHI KUROSAWA, Ayumi Iwata, Yukihiro Satou, Yoshinari Abe, Yasuhito Igarashi, Tomoaki Okuda, *Keio University*

After several years have passed from the Fukushima Daiichi Nuclear Power Plant accident, insoluble radioactive Cs-bearing particles have been found in some regions in Japan. These insoluble particles remain as a particle in human airways and continue emitting radiation. Therefore, there could be a concern about health effects. The particles are seemed to have present in contaminated nuclear reactors and the surrounding areas of F1NPP. To eliminate the hazard of the particles, it is necessary to understand and utilize the physical properties of the particles, which is not elucidated yet.

Because of the continuous emission of the electron beam, we hypothesized that the radioactive particles have specific electrostatic charging characteristics. In this study, we attempt to apply the technique of Kelvin Probe Force Microscopy (KPFM) to measure electrostatic charging characteristics of the particles.

KPFM is a method that enables imaging of nanometre-scale surface topography, and also the surface potential of a sample. KPFM scans a sample with an oscillating probe to detect interatomic force between the probe and the sample. Also, contact potential differences between the probe and sample are detected.

We used a glass substrate for the fixation and measurement medium of the radioactive particles, so we investigated whether the surface potential of the object on the glass substrate could be correctly measured by KPFM. We prepared a glass substrate with partially deposited of Au and biased arbitrary voltage to the Au part. When the bias voltage was changed by 0.1 V from 0.0 V to 0.4 V, the surface potential measured by the KPFM accurately represented the applied voltage.

Also, we measured radioactive Cs-bearing particle by KPFM, and there was the distribution of potential in the surface of the particle. The surface potential of the particle was approximately between +0.3 V and -0.3 V.

2IM.30

Recent Developments and Improvements to a Continuous Flow Diffusion Chamber for Measuring Ice Nucleating Particles. GAVIN MCMEEKING, Ezra Levin, Tim Gordon, Kai Bi, Russell Perkins, Ping Chen, Paul DeMott, *Handix Scientific*

We present a summary of several threads of development focusing on improvement and characterizing the performance of a continuous flow diffusion chamber for measuring ice nucleating particles (INP). Development efforts include work done to improve the refrigeration performance of the instrument, eliminate the need to chemically re-treat the internal surfaces of the instrument, automate all aspects of instrument operation, and reduce measurement artifacts. We include laboratory and field test data for both ambient and previously characterized ice nucleating particle samples, as well as comparisons to existing INP measurement methods. We also discuss in-progress development work focused on producing and testing an improved airborne version of the instrument.

2IM.31

A Variable Residence Hygroscopicity Tandem Differential Mobility Analyzer (VRHTDMA). DEANNA MYERS, James Smith, Jonathan Abbatt, *University of California, Irvine*

Because atmospheric aerosol particles can grow into cloud condensation nuclei, it is crucial to understand how size-selected particles uptake water and the timescale of that process in order to predict their potential climate impacts. In addition, quantifying the timescale and magnitude of water uptake in particles provides insight into particle morphology and phase state, which are important considerations for determining heterogeneous chemical processes. To address these needs, we have developed a Variable Residence Hygroscopicity Tandem Differential Mobility Analyzer (VRHTDMA) to measure the hygroscopicity of aerosol nanoparticles and to provide insights into the timescales of water vapor uptake. The VRHTDMA is a standard HTDMA that can determine hygroscopic growth factors and κ as functions of dry diameter. In addition, this instrument contains four different humidification channels that allow the particles to experience humidification times of 2, 4, 10 and 58 seconds. Results from laboratory characterization experiments are presented. In addition, we present measurements obtained by the VRHTDMA from the OASIS campaign in Utqiagvik, Alaska that demonstrate instrument performance.

2IM.32

Suggested Calibrations for Aerodyne Aerosol Mass Spectrometry to Reduce Uncertainty and to Improve Quantification. BENJAMIN A. NAULT, Hongyu Guo, Pedro Campuzano-Jost, Douglas Day, Jose-Luis Jimenez, *CIRES, University of Colorado, Boulder*

The Aerodyne Aerosol Mass Spectrometry (AMS) is a widely used instrument to measure the chemical composition of submicron, non-refractory particulate matter (PM₁) in real time. The AMS can produce quantifiable speciated mass concentrations and size distributions for numerous species. However, to achieve this, to reduce the uncertainty in the measurement, and to properly interpret comparisons with other measurements, careful calibration of the AMS is necessary. Suggested calibrations have been highlighted during various AMS User's Meetings; however, it could be daunting to find the proper resources to understand what calibrations are necessary, the frequency for the calibrations, and the associated uncertainty by neglecting to perform one type of calibration. Here, we overview the calibrations typically performed for a high-performance aircraft AMS, and break down which calibrations are accessible for most AMS users versus which calibrations can be more challenging. With this, we detail the type of calibrations and the associated uncertainty in neglecting these calibrations. Also, the suggested frequency of calibration, depending how the AMS is being used (e.g., flight AMS and therefore being turned on and off every day versus ground AMS that remains on for extended periods of time), will be discussed. These results will be placed into context of comparisons with other measurements during recent studies.

2IM.33

Investigating Submicron Inorganic Salts Biases Collected on Filters Collected in Airborne Campaigns. BENJAMIN A. NAULT, Pedro Campuzano-Jost, Douglas Day, Jack Dibb, Karl D. Froyd, Eric Scheuer, Jose-Luis Jimenez, *CIRES, University of Colorado, Boulder*

The mass concentration and speciation of accumulation and coarse mode aerosol is important to investigate the chemical and physical processes controlling aerosol from emission sources to the most remote regions of the atmosphere. Collection of aerosol onto filters to be analyzed off-line by chromatography is one technique widely used, especially for analysis of refractory salts (e.g., NaCl, NaNO₃, MgSO₄, etc.), as well as for NH₄NO₃, (NH₄)₂SO₄, and HNH₄SO₄. Here, we use observations collected onboard the NASA DC-8 during recent NASA campaigns. Two substantial differences appear when comparing the submicron inorganic salts measured from filters versus real-time techniques.

First, we find that for an urban study (KORUS-AQ), where NH₄NO₃ is elevated due to anthropogenic emissions of NO_x, nitrate measured from the filters can be lower than the nitrate measured by both AMS and on-line ion chromatography. Data from an airborne thermal denuder suggests that the higher temperatures in the cabin (vs. ambient) may lead to volatilization of nitrate off the filters during handling. A thermodynamic model simulation of this situation confirms that NH₄NO₃ on the filters will quickly volatilize as NH₃ and HNO₃. These results are important for interpreting aircraft results and comparisons when volatile nitrate dominates over non-volatile nitrate, such as East Asia and Europe.

Second, for recent remote studies (NASA ATom), the filters consistently show ammonium-to-sulfate molar ratios of 0.5 (equivalent to NH₄HSO₄) or higher. However, the AMS and a single particle mass spectrometer (PALMS) indicate a larger range of values. With literature values, we show that the substantial uptake of NH₃ onto H₂SO₄ particles on the filters to form NH₄HSO₄ can occur in 20 s or less. Further experiments are being conducted with conditions representative onboard the DC-8 to validate the calculations. These results will allow improved interpretation of ammonium balances from filter and real-time measurements, especially in remote regions.

2IM.34

MFAssignR: Software Tools for Molecular Formula Assignment of Organic Aerosol. SIMEON SCHUM, Lynn Mazzoleni, Laura Brown, *Michigan Technological University*

Recently the use of ultrahigh resolution mass spectrometry has become increasingly popular in aerosol research due to its unparalleled ability to investigate the molecular composition of organic aerosol. Several methods have been developed to work with this data, including commercial (e.g., Composer, PetroOrg) and open source (e.g., Formularity, UltraMassExplorer) options. Open source methods are typically limited to molecular formula assignment based on a database matching approach. Meanwhile, commercial methods are typically capable of performing additional critical steps (e.g., noise estimation, isotope identification and mass recalibration), but they are often expensive and have little transparency regarding the molecular formula assignments. To address these deficits, we developed MFAssignR, an open source software package written in the R programming language available for download via GitHub. The MFAssignR package contains functions for molecular formula assignment, noise estimation, isotope identification, and mass recalibration. In MFAssignR, the molecular formula assignment is done in a data dependent way, meaning a priori decisions about the composition of a sample are not required to significantly decrease the overall assignment ambiguity. In addition, novel methods for noise estimation and isotope identification were developed as part of this package. From our comparison of MFAssignR to several other methods, we found that the MFAssignR assignments are equivalent for the higher intensity peaks and superior for the lower intensity peaks. This is due to the multiple molecular formula extensions used for assignment in MFAssignR. Furthermore, of the peaks commonly assigned, 97-99% were assigned to the same molecular formula. The development of MFAssignR is particularly valuable for organic aerosol research because previous methods, developed for either dissolved organic matter or petroleum samples, contained assumptions that are not appropriate for organic aerosol.

2IM.35

Measurement of Sub 3 nm Flame-generated Particles Using Boosted Butanol CPC 3776 and DEG CPC. GIRISH SHARMA, Mengda Wang, Michel Attoui, Pratim Biswas, *Washington University in St Louis*

Ultrafine laminar TSI CPC is widely used in aerosol science for the detection of particle greater than 3 nm. For the measurement of particles as small as 1 nm, di-ethylene glycol (DEG) booster is used to activate these particles, before they are detected by butanol based CPC. CPC does provide reduction in background noise as compared to electrometer, but suffers from polarity and chemistry dependent activation efficiencies.

In this work, the new half-mini DMA is used to classify particles as small as 1 nm with high resolution. Different types and sizes of ions/particles are generated in sub 3 nm range viz. four different types of tetra-alkyl ammonium bromide ions from electrospray set-up; titanium dioxide nanoparticles using flame aerosol reactor; and soot particle from McKenna burner to study the chemistry dependence of boosted butanol TSI CPC 3776, and TSI DEG CPC. First, the best operating conditions for the boosted CPC are selected which provides maximum signal with minimal noise ($< 10 \text{ \#}/\text{cm}^3$), and were found to be at saturator temperature 45 C, and condenser temperature of 10 C, with capillary flow rate of 70 sccm. These conditions were then set for the measurement of flame generated particles. It is found that negatively charged particles are more easily activated as compared to positively charged for all the particles. Moreover, the activation efficiency is found to be chemistry dependent for mobility size less than 1.8 nm, above which the chemistry dependence was negligible for butanol based CPC. The activation efficiency of different flame generated particles is also compared for DEG CPC.

2IM.37

Analysis of Organic Composition on PM_{2.5} Aerosols by Two-Dimensional Gas Chromatography Mass Spectrometry (GC×GC-MS). JIA-LIN CHARLIE WANG, Neng-Huei Lin, *National Central University, Taiwan*

The objective of this study is to characterize organic constituents on aerosols relevant to their emission sources and the key compounds revealing the evolution of aerosols with the use of a novel analytical technique.

The conventional GC-MS technique has been used to analyze the organic composition of aerosols. However, the high organic complexity of aerosol samples often renders GC-MS technique unsatisfactory in terms of compound separation and identification. As a result, time-of-flight mass spectrometry (TOF-MS) coupled with comprehensive two dimensional GC (GC×GC-TOF) was preferred. A flow type of modulator instead of a thermal type was used in GC×GC as a prelude to field applications without the need of cryogen. The high data sampling rate of 50 Hz for the TOF MS is pivotal to produce very detailed and reproducible GC×GC results. The tolerance of high carrier gas flow rates of up to 5 mL/min played the key role to achieve high sample throughput and thus better sensitivity.

The GC×GC results have been obtained by analyzing both PM₁₀ and PM_{2.5} samples collected by high-volume samplers. By spiking with a known amount of long-chain alkanes as the markers of molecular size, we found that the majority of the organic analytes were in the range of 12 - 30 carbon numbers falling in the category of semi-volatile organic compounds (SVOCs). If excluding alkanes, 45 and 56 compounds of alcohol, aldehyde, ketone, and ester varieties were able to be tentatively identified for the PM₁₀ and PM_{2.5} samples (see the figure below for an example of a PM_{2.5} sample), respectively, which are mostly primary organic aerosols (POA). Intriguingly, trace amounts of plasticizers and phosphorus flame retardants were also found. Compounds such as these are unique to the specific sources, called markers, demonstrating the wide spread of these hazardous compounds in the environment.

2IM.38

The Comprehensive Thermal Desorption Aerosol Gas Chromatograph (cTAG) for Consistent Quantification of VOCs, IVOCs and SVOCs. REBECCA WERNIS, Nathan Kreisberg, Robert Weber, Susanne Hering, Allen Goldstein, *University of California, Berkeley*

Aerosols are a source of great uncertainty in radiative forcing predictions and have poorly understood health impacts. Most aerosol mass is formed in the atmosphere from reactive gas phase organic precursors, forming secondary organic aerosol (SOA). Semivolatile organic compounds (SVOCs) (effective saturation concentration, C^* , of 10^{-1} - 10^3 $\mu\text{g}/\text{m}^3$) comprise a large fraction of organic aerosol, while intermediate volatility organic compounds (IVOCs) (C^* of 10^3 - 10^6 $\mu\text{g}/\text{m}^3$) are abundant and efficiently react to form SOA. VOCs ($C^* \geq 10^6$ $\mu\text{g}/\text{m}^3$) are precursors to SOA with high reactivity, abundance, and impacts on ozone formation.

The Comprehensive Thermal Desorption Aerosol Gas Chromatograph (cTAG) is the first single instrument sensitive to compound-specific VOCs, IVOCs and SVOCs. 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 coupled to a single High-Resolution Time-of-Flight Mass Spectrometer, achieving consistent quantification across 14 orders of magnitude of vapor pressure. cTAG obtains concentrations hourly and gas-particle partitioning for SVOCs bihourly, enabling observation of the evolution of these species through oxidation and partitioning into the particle phase. Online derivatization for SVOCs enables detection of polar and oxidized species.

In this work we present design details and data evaluating key parameters of instrument performance such as detection limits, measurement uncertainties, and linearity and reproducibility of calibration curves obtained using a custom liquid evaporation system for I/VOCs. VOC measurements are compared with a collocated GC-FID system performing routine VOC monitoring. Example timelines of precursors with secondary products are shown. Based on known chemical tracers and temporal correlations between measured compounds, we present the initial findings to elucidate the relative contributions of pollution sources to PM_{2.5} in Livermore, CA during spring 2018.

2IM.39

A Quadrupole Electrodynamic Trap Coupled to Single Droplet Mass Spectrometry: A Tool to Study Aerosol Heterogeneous Reactivity. MEGAN WILLIS, Grazia Rovelli, Kevin Wilson, *Lawrence Berkeley National Laboratory*

Trapping and levitation of single particles has become an important tool to investigate the physical and chemical properties of aerosol particles under controlled laboratory conditions. Particle levitation provides access to heterogeneous chemistry at atmospherically relevant conditions through reaction timescales of hours to days and, correspondingly lower oxidant concentrations compared to shorter reaction timescales. Chemical evolution in trapped particles can be followed using spectroscopic techniques; however, these approaches are not amenable to all atmospherically relevant chemical systems. We couple a linear quadrupole electrodynamic trap (QET) to single droplet mass spectrometry to probe the chemical evolution of the condensed phase due to heterogeneous reactions on populations of trapped droplets. The multi-compartment QET is housed in an environmentally controlled chamber and allows for continuous trapping of a droplet population (~10 – 100 droplets). Single droplets are transferred to a lower compartment for sizing using the Mie scattering pattern from illumination by a 532 nm laser introduced axially. Single droplets are subsequently ejected to the ionization region of an ambient pressure inlet mass spectrometer. We extend previous work using paper spray mass spectrometry coupled to a branched QET (Jacobs et al., 2017), to the use of electrospray ionization (ESI) and solvent-assisted inlet ionization (SAII). Our aim is to establish a reproducible and quantitative method for detecting organic compounds, and their reaction products, in single micron sized aqueous or pure component droplets. We explore the time resolution required to capture and quantify droplet events using ESI and SAII, and the sensitivity of these two approaches as a function of droplet size, concentration and charge. We develop the use of droplet internal standards inert to reaction with the chosen oxidant to improve the reproducibility of droplet detection. Finally, we study the ozonolysis of organic acid alkenes, and examine the interchangeability of reaction time and oxidant concentration.

Jacobs et al. (2017). *Anal. Chem.*, 89(22), 12511–12519.

2IM.40

Ambient Measurements of Emissions from Biomass Combustion Using a Portable Measurement Backpack. MARILYN WURTH, Brian P. Frank, Jake Lindberg, Nicole Vitillo, Patricia Fritz, Shida Tang, Gil H. LaDuke, David Guerrieri, *New York State Dept. of Environmental Conservation*

Laboratory and ambient evaluations of emissions from some advanced biomass (wood) combustion devices indicate ultrafine particle (UFP) emissions from these devices may be significant in rural areas. This research consisted of source and ambient measurements of a high efficiency, two-stage wood gasification boiler under typical homeowner operational conditions to complement previous stack measurements of various advanced wood combustion devices (emissions diluted approximately 100:1) during controlled laboratory test methods.

A novel measurement method utilizing portable instrumentation measuring PM₁₀, PM_{2.5}, PM_{1.0}, (DRX 8530, TSI Inc.), UV-IR black carbon (microAeth® MA300, AethLabs), UFP particle number concentration (PNC) (Personal Ultrafine Particle Counter, Enmont, LLC), and lung deposited surface area (LDSA $\mu\text{m}^2/\text{cm}^3$) (Partector, Naneos, Inc.) was carried on a backpack to survey personal exposure to ambient emissions within a 100 ft radius of the source. This radius was defined by New York State Department of Environmental Conservation setback requirements for residential-size new outdoor wood boilers or hydronic heaters to reduce air quality impacts to nearby residences. Source stack emissions were measured concurrently for similar parameters and included particle size distributions and size-segregated samples. Preliminary ambient data shows sustained, elevated UFP PNC were measured within the 100 ft radius. The average ambient PNC was greater than average PNC found within 100 ft of a near roadway environment in an environmental justice community. However, the average LDSA measured near the wood combustion source was substantially less indicating a larger particle size distribution above the Partector's range (20-400 nm). These results may help inform public health exposure assessments applicable to different community settings in urban and rural areas.

2IM.41

Application of Synchrotron Radiation for the Morphology and Internal Structure of Individual Aerosols. Chao-Wei Lai, Yu-Han Chen, Wan-Yi Chen, Chun-Chieh Wang, Yao-Tung Lin, LI-HAO YOUNG, *China Medical University, Taiwan*

The morphology of aerosols affects their transport, optical and hygroscopic properties. This study aims to utilize synchrotron-based transmission X-ray microscopy (TXM) 2D radiography and 3D tomography to identify the particle size, shape and internal structure of individual aerosols. Size-fractionated (2.5, 1, 0.5 and 0.25 μm) ambient aerosols were collected on transmission electron microscopy (TEM) grids, which were then subjected to TXM analysis at the National Synchrotron Radiation Research Center (NSRRC) in Taiwan. TXM 2D images were collected with 60s exposure time and a spatial resolution of about 60 nm. Subsequently, 3D images were reconstructed using sequential projections taken with the azimuth angle rotating from -90° to $+90^\circ$. Transmission/scanning electron microscopy (TEM/SEM) images were also taken for comparison. Preliminary results show that the aerosols exhibited spherical, aggregate, rod, polygon and irregular shapes. More importantly, the synchrotron-based TXM 2D/3D images can reveal the complex internal structure of aerosols, including solid, porous, hollow or core-shell, that are not visible by TEM/SEM. In addition, heavy elements were found to be more associated with spherical aerosols. The outputs of this study provide us with new insights of the potential origin, formation mechanisms and aging processes of ambient aerosols.

2IM.42

Ultrafine Particles – Effects of Aerosol Material on Different Nanoparticle Counters. AXEL ZERRATH, Andrea Tiwari, Patrick Roth, *TSI Incorporated*

Atmospheric aerosol particles are quantified using different technologies, each of which focuses on a certain size range of particles. The number concentration of ultrafine particles is usually measured by Condensation Particle Counters (CPCs), while Mobility Particle Sizers are able to determine the size distribution.

CPCs utilize a condensation process to grow the nanoparticles into droplets, which makes them visible to counting optics. Different types of working fluids can be used in this growth process; the most commonly used liquids are butanol and water. In environmental and indoor air quality studies water-based CPCs have gained much attention due to the fact that use of organic solvents is avoided and distilled water is used instead. Under typical ambient conditions both liquids are able to activate and grow airborne aerosol particles identically.

However, at the small particle size threshold of an instrument, the activation process can be influenced by the chemical composition of the aerosol particle. This is a consequence of the chemical and physical interaction between the aerosol material and the working fluid. For this reason the so-called detection efficiency (efficiency with which particles of a given size are successfully detected) for small aerosol particles (typically smaller than 20 nm) needs to be investigated as a function of both aerosol chemical composition and type of working fluid.

In this study we present data focusing on the counting efficiency of various aerosol materials comparing a new water-based nanoparticle counter to the latest generation of butanol-based CPCs.

This study will also present size distribution measurement comparisons between butanol- and water-based systems, when challenged with laboratory model aerosols as well as urban air atmospheric aerosols.

2IM.43

Imaging Aqueous Submicron Particles through the Development of a Flash Freeze Technique. THERESA KUCINSKI, Miriam Freedman, *The Pennsylvania State University*

Understanding aerosol effects on Earth's climate is dependent on particle characterization which requires the development of new analytical techniques. In particular, methods to study morphology and phase are needed to encompass a broad size regime that can range from nanometer to micrometer particles. It is also crucial to include the study of morphology in relation to relative humidity (RH) to be able to predict the phase state of aerosol particles in the atmosphere. Particles can undergo liquid-liquid phase separation (LLPS) with cycling humidity levels and the resulting phase state can alter the physics and chemistry of aerosol particles in the atmosphere. Furthermore, it has been shown that LLPS is size dependent in the submicron range when imaging dried particles. LLPS has been well documented at the micrometer scale through the use of optical microscopy that allows for imaging of particles over a range of RH values. However, studies of phase separation in aqueous submicron particles over a range of RH remain elusive due to limitations of current techniques. We developed a flash freeze technique to capture submicron particles through a range of RH values and image via cryogenic transmission electron microscopy (cryo-TEM). The method is similar to the vitrification technique found in biosciences but instead utilizes a temperature controlled flow tube that vitrifies particles equilibrated at a chosen RH. The flash freeze method allows for imaging of aqueous multicomponent aerosol particles at multiple points in the phase transition region. With this technique, we have characterized the phase transition region for the following multicomponent systems: 2-methylglutaric acid/ammonium sulfate, 1,2,6-hexanetriol/ammonium sulfate, and a complex organic mixture/ammonium sulfate. These characterizations provide new insight into the process of LLPS for submicron aerosol particles.

2IM.44

Transmission of Charged Nanoparticles through an Adverse Axial Electric Field and Its Improvement. RUNLONG CAI, Jingkun Jiang, *Tsinghua University, China*

In aerosol studies, it is often encountered that charged nanoparticles or ions are transported against an adverse electric field. For instance, when classifying them according to their electrical mobility using a differential mobility analyzer (DMA), charged particles usually have to migrate against the adverse electric field in the sample outlet (or inlet in some cases). An analytical solution for the transmission efficiency of non-diffusive particles through the adverse electric field was proposed by Tammet (2015), which agrees well with experimentally measured transmission efficiencies. For sub-10 nm particles, diffusional losses are usually non-negligible when estimating the transmission efficiency through a tubing. In this study, we proposed an analytical model for estimating the transmission efficiency of charged nanoparticles (and ions) through an adverse axial electric field. Particle losses due to diffusion and electrostatic migration are both considered. Particle concentration profile at the cross-section of the tubing exit is calculated by solving the Graetz problem when neglecting particle electrical migration, then the effect electrostatic losses is coupled to this concentration profile using the method proposed by Tammet (2015). The transmission efficiency is shown to be a function of only two dimensionless parameters that characterize particle diffusion and electrostatic migration, respectively. The proposed analytical model was applied for an electrical mobility filter and the sample outlet of a differential mobility analyzer. The transmission efficiency estimated using the analytical model agrees well with those simulated using a Monte Carlo method and experimentally measured transmission efficiencies for sub-6 nm particles. For the tested conditions, the mean absolute difference between the transmission efficiencies estimated using the analytical model and the simulated efficiencies is 0.8%.

The transmission efficiency of nanoparticles through a miniature cylindrical DMA was improved using this analytical model. A DMA sample outlet made of electrostatic dissipative tubing was used to reduce the adverse electric field intensity. Although the flow field and particle diffusion in a real DMA sample outlet are usually complex, we found that the length of the electrostatic dissipative tubing corresponding to relatively high transmission efficiency in typical conditions can be practically determined using a rough criterion: the length is recommended to be longer than a threshold value such that the ratio of particle electrostatic migration velocity to average air flow velocity is smaller than 0.2. Compared to the Delrin insulator which was conventionally used at the DMA sample outlet, the new electrostatic dissipative sample outlet increased the penetration efficiency of ~1.5 nm ions by 30-50% in a typical operating condition.

2IM.45**Lab-based Test of Palm-sized Aethalometer for Indoor Aerosol Measurement.** JEONGHOON LEE, *KOREATECH*

Despite versatile use of a small aethalometer at various research fields such as black carbon measurements and personal exposure studies, it is difficult to find the information about how the palm-sized aethalometer performs. Encouraged by this, a real-time test was carried out using indoor aerosol to provide performance characteristics for proper usage. According to the preliminary results, the palm-sized aethalometer exhibited excellent performance at some conditions though it showed poor performance sometimes, for example, when the device was directly connected to a power adapter. Another example includes the production of negative values under low concentration conditions. It is important to note that a verification process before use may be required at a certain condition. Toward this, 10 days long consecutive test was performed. Attenuation value (ATN) calculated from the reference signal and the measured signal was monitored and compared with the recorded attenuation. A discussion including more detailed explanation will be presented regarding what caused poor performance of the palm-sized aethalometer.

2IM.46**Real-Time Measurement of Airborne Carbon Nanotubes.** Lina Zheng, PRAMOD KULKARNI, *Centers for Disease Control and Prevention, NIOSH*

With growing applications of carbon nanomaterials, there is a concern over health risks presented by inhalation of carbon nanotube (CNT) aerosol in workplace atmospheres. Current methods used for CNT aerosol measurement lack selectivity to the specific form of carbonaceous component or allotrope of interest. Moreover, the detection limits of these methods are also inadequate for short-term monitoring. Here, we describe, for the first time, a near real-time, field-portable instrument for selective quantification of airborne CNT concentration. The approach uses an automated cyclical scheme involving collect-analyze-ablate steps to obtain continuous near real-time measurement using Raman spectroscopy. The method achieves significantly lower detection limits by employing corona-assisted particle microconcentration for efficient coupling with laser Raman spectroscopy. A combination of techniques involving: i) use of characteristic Raman peaks, ii) distinct ratio of disordered and graphitic peaks, and iii) principal component classification and regression is employed to identify and quantify the specific form of the aerosolized carbonaceous nanomaterial. We show that the approach is capable of selectively quantifying trace single-walled CNT in the presence of interferences such as diesel particulate matter. The detection limit of the method for single-walled CNTs was 60 ng m^{-3} , corresponding to a 10-min aerosol collection period, which is significantly lower than that for the NIOSH Method 5040 ($\sim 0.15 \text{ } \mu\text{g m}^{-3}$ for an 8-hour collection on a 25-mm filter at 4 L min^{-1}), a commonly used method for elemental carbon. We demonstrate the automated real-time capability of this field-portable method by continuously measuring a transient single-walled CNT aerosol.

2IM.47

An Exhaled Breath Aerosol (EBA) Collector for High Collection Efficiency of Particles Down To 10nm. ARANTZAZU EIGUREN FERNANDEZ, Gregory Lewis, Susanne Hering, Somayeh Youssefi, Donald Milton, *Aerosol Dynamics Inc*

The new ice-impacting (icePAC) Exhaled Breath Aerosol Collector (EBAC) was developed for efficient collection of particles and proteins exhaled by a subject person. The EBAC takes advantage of the vapor-saturated nature of the exhaled breath to enable condensational growth and concentrated collection of particles down to 10nm onto an ice substrate. Exhaled breath flows through six wick-lined parallel tubes maintained at 0°C, subsequently passing through a delivery nozzle, and impinges onto a sample collection plate maintained at approximately -14°C. Enlarged particles are deposited by impaction onto an ice-covered surface. The cold tubes serve two purposes: 1) due to the non-linearity of the water vapor pressure curve, water condenses on particles in the exhaled breath causing them to grow above 1 micrometer allowing collection by impaction; and 2) removal of the water vapor condensed on the wick walls, concentrating the collected sample. The new EBAC was tested in the laboratory using test aerosols to optimize sampling conditions for highest collection efficiency. Relative humidity of the incoming flow, particle size and sampling time were some of the parameters evaluated. Collection efficiency was highly dependent on the RH of the sampling aerosol. Low efficiencies were measured for RH <75%, increasing rapidly with increasing RH, and reaching 85-90% at RH=85%. At RH=90% both ambient and sulfate particles were collected with efficiencies higher than 95%. For particle size dependency, collection efficiencies higher than 90% were measured for particles $D_p > 10\text{nm}$, decreasing to ~80% for particles down to 8 nm.

Collection efficiency under optimized conditions was also tested by chemical analysis. Results for the EBAC compared with a sequential spot sampler suggested that losses into the delivery nozzle were minimal, with high collection efficiencies onto the ice collection surface. In summary, the collection efficiency of the EBAC is about 90% when considering both physical and chemical collections.

2IM.48

Orthographic Imaging of Free-Flowing Aerosol Particles. JESSE LANING, Matthew Berg, *Kansas State University*

A method to obtain contact-free images of aerosol particles with digital holography from three orthogonal directions without lenses. The approach uses three diode lasers of different wavelengths to simultaneously illuminate flowing particles and form holograms on three sensors. Images of the particles are then reconstructed from the holograms and used to infer the three-dimensional structure of the particles. The apparatus employs inexpensive components and requires no lenses to achieve the imaging, giving it a large sensing volume and simple design. Test cases are presented with spherical glass particles and nonspherical pollen particles. The next step for this work is to test more formal techniques, such as weighted back-projection, to better render the 3D form of the particles.

2IM.49

Development of a New Dilution System for Continuous Measurement of Particle Concentration in the Exhaust from a Coal-fired Power Plant. Dongho Shin, Kee-Jung Hong, Hak-Joon Kim, Bangwoo Han, YONG-JIN KIM, *Korea Institute of Machinery & Materials*

The particle concentrations in the exhausts from coal-fired power plants have received much attention because coal-fired power plants are among the largest sources of particulate matter (PM) emissions in Korea. We developed an ejector-porous tube diluter to suppress particle nucleation and minimize particle loss. To measure fine particles in a stack continuously, clean air was periodically supplied at high pressure in the diluter. The particle concentrations in the exhaust from a coal-fired power plant in Korea were measured and compared with results obtained using an existing commercial diluter which is a porous tube-ejector diluter. Both the commercial diluter and our diluter successfully suppressed the particle nucleation of volatile compositions, which commonly happens at cold dilutions of hot gases. However, the commercial diluter showed significant particle losses in the PM_{2.5}–10 size range, whereas our diluter did not. The diluters developed in this study were installed at two coal-fired power plants to continuously measure the exhaust PM₁₀ and PM_{2.5} for a long time. Using the optical particle counter (OPC, 1.109, Grimm, Germany) with the diluter developed in this study, we measured the size distributions for mass concentrations at two coal-fired power plants and the measured PM₁₀ were compared with the gravimetric method (EPA M201A) which is a standard method for measuring the PM₁₀. The relative accuracies between our method and the EPA M201A were less than 20%, a suitable value for continuous monitoring PM₁₀ in stacks. 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 (Grant No. 20161110100140).

2IM.50

Development of a Novel Particle Mass Spectrometer for Online Measurements of Refractory Sulfate Aerosols. YUYA KOBAYASHI, Yu Ide, Nobuyuki Takegawa, *Tokyo Metropolitan University*

Sulfate aerosols are ubiquitous in the atmosphere. Ammonium sulfate (AS) is generally the dominant form of sulfate aerosols in urban air, whereas sodium sulfate (SS) and potassium sulfate (PS) may have large contributions in remote areas. Currently available methods for online measurements of sulfate aerosols, which are based on ion chromatography (IC) or thermal desorption aerosol mass spectrometry, cannot separately quantify nonrefractory and refractory sulfate compounds. We have developed a new particle mass spectrometer to measure nonrefractory and refractory sulfate compounds. Aerosol particles are introduced into a vacuum chamber via an aerodynamic lens unit and are collected on a thin graphite plate. To reduce loss of particles due to bounce on the plate, aerosol particles are coated by condensation of oleic acid vapor prior to the sample inlet. A focused CO₂ laser coupled with the graphite plate enables high desorption temperature (black-body equivalent temperature of ~1000 K) for detecting AS, SS, and PS aerosols. The gas molecules evolved from these compounds are detected using a quadrupole mass spectrometer. The key parameters of the condensation growth tube for oleic acid coating (e.g., temperature, tube length) were optimized in the laboratory. The response of the instrument to monodisperse AS, SS, and PS particles was also tested in the laboratory. While a good linearity was found for these compounds, the sensitivity for PS exhibited smaller values compared to the other compounds. Possible thermal decomposition processes of AS, SS, and PS are discussed based on the fragment ratios of these compounds. We propose a method to separately quantify AS, SS, and PS mass concentrations from mixed particles containing these compounds.

2IM.51

A Test and Evaluation (T and E) Capability for Aerosolised Hazardous Materials. SARAH MARCHANT, Peter Jones, Will Sellors, Maurice Walker, Andy Martin, Buckley Margaret, *Dstl, Porton Down, Salisbury, Wiltshire, SP4 0JQ, UK*

Introduction

A chemical aerosol Test and Evaluation (T&E) facility has been designed and built at Dstl, Porton Down that allows the reproducible generation of aerosols of hazardous chemicals. This has involved undertaking a detailed safety investigation to ensure there was no risk to the operator, observers or environment. The aim has been to design a T&E facility that can safely test detection systems against toxic chemical aerosols in a 'dial-up' manner for prolonged test periods.

Experimental Method and Results

The chemical aerosol test facility has been installed at Dstl, Porton Down and it enables the robust, reliable and reproducible T&E of aerosol detection technologies. This provides an understanding of the potential of such detection technologies to meet the needs of future requirements. The chemical aerosol test facility is constructed of stainless steel tubing with aluminium gaskets and has a total length of 1600 mm. A novel method of aerosol generation is presented that produces particles of the hazardous chemicals with a size range of 0.25 μm to 3 μm . The system runs at a negative pressure (-1.5 mbar) to minimise the potential of leaks and the total aerosol concentration can be tuned over a relevant dynamic range. Chemical sensors can be connected to the flow tube and their performance against the aerosolised chemicals can be assessed. The aerosol concentration within the flow tube is constantly monitored using a Grimm Mini-LAS 11.R and this is confirmed off-line with DAAMS sample tubes analysed by LC-MS.

Conclusions

This work has led to the safe generation of aerosols of hazardous materials (including Chemical Warfare Agents). These aerosols can be generated at a stable concentration for up to two hours and have been confirmed by off-line analysis. Currently, Dstl is using this capability to generate test aerosols for the T&E of prototype Chemical Detection equipment.

2IM.52

A Comprehensive Isomeric Identification of Particle-Phase Organic Nitrates by Gas Chromatography and Time-Of-Flight Mass Spectrometry Coupled with Electron Capture Ionization. XIAODI SHI, Xinghua Qiu, *Peking University*

Organic nitrates (ONs) are important composition of secondary organic aerosol (SOA) serving as the reservoir or sink of NO_x. However, little information is available in urban area of developing counties characterized by high anthropogenic VOCs emission. Chemical composition of ONs in these area is crucial to uncover their formation mechanism. But current methods couldn't meet the demand on individual or isomeric identification of ONs. In this study, a method based on gas chromatography/ electron capture negative ionization tandem time-of-flight mass spectrometry (GC/ECNI/ToF-MS) was established to comprehensively identify unknown ONs in PM_{2.5} sampled in Beijing. Under ECNI condition, ONs can cleavage into NO₂⁻, [M-NO₂]⁻, [M-NO₂-H₂]⁻. NO₂⁻ can be used as an indicator of ONs and another pair of ions can provide element composition. Deconvolution was performed and ONs were filtrated according to fragment rules after analyzing organic extracts of PM_{2.5} in full scan mode. 81 features were recognized as potential ONs. And 12 features were verified by the synthesized authentic standards. Potential ONs were composed of arylalkyl nitrate and hydroxy nitrate generated from styrene, alkenes and biogenic VOCs. Isomers of hydroxy nitrate formed from 1-alkenes were confirmed by synthesized authentic standard. Isomeric distribution was used to reveal the relative contribution of daytime and nighttime formation mechanism. High abundance of ONs with nitrate group located at α position suggesting that night formation mechanism was predominant. This method provides information on the individual species of ONs and can enhance our comprehension of the formation mechanism.

2IM.53

Development of a Direct-Reading Inhalable Particle Sizer with Elemental Composition Analysis. JAMES SIPICH, John Volckens, Christian L'Orange, Azer Yalin, Kimberly Anderson, Christopher Limbach, *Colorado State University*

No technology currently exists to quantify the size and elemental composition of large (>20 μm) airborne particles in real time. Such aerosols are created from manufacturing processes such as abrasive grinding and cutting; they are also present following mechanical resuspension (i.e. wind-blown dust). Exposure to large, inhalable aerosols can have a substantial detrimental impact on health. Our understanding of the behavior of such particles is limited, due in part to a lack of information about their size and elemental composition. Current methodologies for characterizing inhalable particles involve sample collection onto filter substrates that require subsequent offline analyses. These provide only time-integrated results, which further limits our ability to study the dynamic nature of aerosols. A device capable of directly measuring the size and composition of large particles would be a valuable tool for the identification and control of occupational aerosol hazards.

The objective of this work was to develop a portable, direct-reading instrument to determine the size and composition of airborne particles larger than 20 μm in aerodynamic diameter. Particle size is determined by analyzing the light signals produced as a result of Mie scattering as settling particles pass through an infrared laser sheet. The current prototype device can detect and size particles from 20 to 130 μm , though this detection range can be adjusted. Chemical composition of particles is established through laser induced breakdown spectroscopy (LIBS) that immediately follows the Mie scattering measurement. The LIBS process uses a pulsed laser source to form a plasma that excites the electrons in the material within the plasma. As these electrons relax, light is emitted at characteristic wavelengths that depend on the elemental composition of the analyte mass. The prototype device can perform simultaneous detection of light emitted in the 300-800nm range, sufficient for LIBS analysis of many common materials.

2IM.54

Assessment of Acrolein in Air Samples Using Pentafluorophenylhydrazine (PFPH) and Gas Chromatography-Mass Spectroscopy (GC-MS). Anthony Cutler, TOKALA CHRISTENSEN, Jenna Nelson, Hansina Hill, Odelle Hadley, Robin Bond, *The Evergreen State College*

Acrolein is a respiratory irritant and common Hazardous Air Pollutant (HAP) emitted during combustion. Anthropogenic and natural sources include cooking meat and oil, residential wood and oil heating, diesel combustion and wildfires. Due to potential impacts on public health, accurately measuring acrolein concentrations in ambient air is a high priority. The Environmental Protection Agency (EPA) uses Method TO-15 to quantify ambient acrolein concentrations. Method TO-15 collects air samples in Summa canisters which are subsequently analyzed with Gas Chromatography-Mass Spectroscopy (GC-MS). This method may produce significant positive biases due to interferences during analysis, as well as discrepancies in canister cleaning and turn-around time between sample collection and analysis. The Eastern Research Group (ERG) provides air toxics sample analysis for the EPA and currently identifies the acrolein Method Detection Limit (MDL) to be 0.120 ppbv (0.28 $\mu\text{g}/\text{m}^3$). This is 14 times higher than the EPA's inhalation reference concentration (RfC) for safe levels of acrolein in air (0.02 $\mu\text{g}/\text{m}^3$). Previous studies have demonstrated that Tenax-TA sorbent coated with pentafluorophenylhydrazine (PFPH) as a derivatizing agent and followed by GC-MS analysis produces low MDLs and may be effectively used to quantify ambient carbonyl concentrations. This study presents the development of a PFPH/GC-MS method specifically optimized for acrolein analysis. The air sample collection tubes were designed to be compatible with the Xontech 925 carbonyl sampler. The Xontech 925 was collocated with a Xontech 910, used for canister sampling, in Lacey, WA between summer 2018 and 2019. The canister samples were analyzed by ERG following Method TO-15. Acrolein samples collected in summer 2019 and analyzed using the new method were compared and evaluated against results obtained from ERG.

2IM.55

Experimental Studies of the Dynamics of Organic Iodide Species Adsorbed on the Surfaces of Environmentally-relevant Particles. ALLA ZELENYUK, Robert VanGundy, Katarzyna Grubel, Thomas Autrey, Youngsoon Shin, *Pacific Northwest National Laboratory*

Nuclear accidents, like Fukushima, can result in a release of harmful radioactive materials, including semi-volatile organic iodides, into the environment. These species are often adsorbed to different surfaces, such as dust or soot particles, or onto sorbents, designed for their efficient capture. A large number of previous studies have been focused on the efficiency and stability of sorbents to trap different iodide species; however, little is known about the chemical and physical transformations of these species with time and due to exposure to real-world conditions, e.g. relative humidity, light, and oxidants.

We will present the results of a recent study, in which we utilize our approaches for real-time separation and multidimensional characterization of individual particles to quantify the rates of transformation of organic iodide species, adsorbed on to the surfaces of graphitic and activated carbon particles and mesoporous silica.

Segregated particles with well-defined properties (mass, size, shape, morphology, porosity, and composition) were introduced into the adsorption/reaction chamber, where they were exposed to semi-volatile iodide-species, e.g. butyl-iodide (Bul). Single particle mass spectrometer, miniSPLAT, was used to quantify adsorption kinetics of iodide species by measuring, in real-time, changes in particle properties (i.e. composition, mass, and density). In addition, these particles were exposed to water vapor, ozone, OH, and UV light, providing information on the chemical transformation of the adsorbed iodide species.

To compare the evolution of chemisorbed and physisorbed organic iodide species, carbon and silica particles were impregnated with DABCO (1,4-diazabicyclo[2.2.2]octane). The data for Bul physisorbed on bare carbon particles, indicate identical temporal evolution of the iodinium and the butyl fragment ions as a function of the exposure time. In contrast, adsorption of Bul on DABCO-impregnated carbon particles exhibit fast physisorption of Bul and the formation of non-volatile mono-substituted DABCO at a slower rate.

Furthermore, to determine binding energies particles with adsorbed iodide species were introduced into temperature-controlled flow tube reactor, which is used to conduct single-particle desorption studies. These measurements were complemented by the traditional batch measurements utilizing temperature programmed desorption mass spectroscopy.

2IM.56

Quantifying Exposure to Second Hand Tobacco Smoke in the Presence of Black Carbon via DualSpot Corrections to MicroAeth Data: Results from Chamber Experiments. ABDERAHIM SALHI, James Ross, Beizhan Yan, Qiang Yang, Jeanine D'Armiento, Jarrod Sonnett, Matthew Perzanowski, Steven Chillrud, *Hudson County Community College; LDEO of Columbia University*

Second hand tobacco smoke (SHS) is associated with an array of adverse health effects making it an important exposure to measure. However, significant shortcomings exist for current methods such as self-reported questionnaires, cotinine/nicotine biomarkers, and airborne tracers such as nicotine. Multi-wavelength absorption methods of integrative filters collected over days to weeks have been promoted but are significantly impacted when moderate to elevated black carbon (BC) loadings are present, which suppress the ultraviolet (UV) signature of the biomass particulate matter (PM). The multi-wavelength microAeth MA350 (AethLabs) includes the option for carrying out DualSpot™ loading corrections on each wavelength-based absorption on highly time resolved data. DualSpot corrections for black carbon have been evaluated through comparison to *in situ* BC methods such as photoacoustic extinctions. As far as we are aware, no-one has evaluated DualSpot corrections under controlled conditions for biomass smoke sources such as SHS. Our chamber experiments mixed SHS from a cigarette machine with ethylene-based BC soot from an inverted flame source to characterize the loadings necessary to suppress the uncorrected UV signature. Then DualSpot corrected data are compared to uncorrected data to evaluate the correction under controlled conditions of near-constant inputs of SHS and BC over time. Black carbon loading significantly suppresses the uncorrected SHS signal starting at around 2 IR ATN units, reaching a suppression of ~40% by 8 IR ATN units. DualSpot correction appears to completely remove the loading effect of BC on the optical signature of SHS as long as the unit has good flow control, with flow on spot 1 (100 ml/min) needing to be 2.0 times that of the flow on spot 2 (i.e. 50 ml/min). Future work should focus on gravimetric calibration of the $\hat{\tau}$ UVPM signature of SHS through collection of filters.

2RA.1

Integrating Aerosol Size Distribution Measurements with a 3D Chemical Transport Model. DANA MCGUFFIN, Peter Adams, Erik B. Ydstie, *Carnegie Mellon University*

Accurately modeling aerosol dynamics is required to obtain an understanding of the particle number size distribution (PNSD), cloud condensation nuclei (CCN) activity, and therefore aerosol indirect effects. Any uncertain processes or uncertain model inputs will lead to uncertainty in the predicted concentration fields. Key uncertainties in predicting CCN concentration fields include formation of primary particles due to aerosol emissions and the nucleation of condensable vapors as well as formation of secondary particles due to the condensation of volatile organic compounds.

The goal of this work is to improve 3D Chemical Transport Model (CTM) predictions by constraining several uncertain dynamics with a network of ground-based PNSD measurements. The CTM utilized here is GEOS-Chem TOMAS using meteorological fields from the Goddard Earth Observing System (GEOS) Data Assimilation System. The model is run with a nested grid over Europe, where European Supersites for Atmospheric Aerosol Research (EUSAAR) has locations measuring the PNSD. We aim to constrain the primary organic aerosol (POA) emissions, nucleation rate, and secondary organic aerosol (SOA) production rates over this region to improve predicted concentration of CCN.

We use a stability-based inverse model previously developed for a box model that estimates POA emission, nucleation, and SOA production rates based on measured values calculated from an observed number size distribution. This method transforms the full PNSD into three summary metrics, each of which are sensitive to one of the uncertain process rates we aim to constrain. In this work, we distribute the inversion technique among each grid block in the 3D CTM that contains a EUSAAR measurement site.

We evaluate the limitations of applying the inverse model based on nonlinear control theory to a CTM. Additionally, we will analyze the error between the estimated and measured PNSDs as the error in the three summary metrics approach zero.

2RA.2

Polarimetric Measurement Sensitivities for Atmospherically Processed Brown Carbon Aerosol. CHENCHONG ZHANG, William Heinson, Benjamin Sumlin, Michael Garay, Olga Kalashnikova, Rajan K. Chakrabarty, *Washington University in St. Louis*

Biomass burning is an important source of brown carbon (BrC) aerosol emissions, which significantly modulate regional atmospheric radiative forcing by strongly absorbing in the near-UV solar spectrum. Because they are partially soluble in water droplets, these particles also affect cloud microphysical characteristics. Multiangle spectropolarimetric remote sensing techniques have proved very useful in characterizing the properties of the atmospheric BrC, including its composition and particle vertical distribution.

Freshly emitted BrC aerosol has been shown to quickly undergo atmospheric processing, changing its optical and physicochemical properties on time-scales ranging between minutes to hours. Current remote sensing retrieval algorithms fail to take these changes into consideration in their parameterizations of BrC aerosol microphysical properties during atmospheric processing. Here, we propose forward modeling to quantitatively analyze the sensitivity of remote sensing parameters to changing BrC aerosol properties as a function of atmospheric processing. We track the evolution of BrC aerosol after emission by configuring the atmospheric layers in a numerical model with aerosols of different aging stages. In this way, the spectropolarimetric pattern of BrC aerosol can be tracked over a long time-scale. Our forward modeling results will be validated with observational data collected by the Jet Propulsion Laboratory's Airborne Multiangle SpectroPolarimetric Imager.

2RA.4

Concentrations of Biogenic Volatile Organic Compound in an East Coast Forest, and Their Relative Importance for Ozone Chemical Loss. DEBORAH MCGLYNN, Chenyang Bi, Graham Frazier, Sally Pusede, Gabriel Isaacman-VanWertz, *Virginia Tech*

Biogenic volatile organic compounds (BVOCs) comprise a significant majority of reactive carbon in the atmosphere. Atmospheric oxidation of BVOCs leads to the formation of secondary organic aerosols and may form or destroy ozone depending on the chemical conditions. Aerosols and ozone can go on to influence ecosystem function, leading to complex atmosphere-biosphere interactions and feedbacks that lead to uncertainties in modeling and long-term predictions. To address gaps in long-term measurements of BVOCs and to understand these interactions, we deployed a custom built, field deployable, VOC-GC-FID at a research tower near Charlottesville, VA. Plant emissions from all major terpenoid classes (i.e. isoprene, monoterpenes, and sesquiterpenes) were measured in and above the canopy of a forest typical of the Appalachian region (mixed deciduous and conifer). Isomer-resolved concentrations were measured with hourly time resolution beginning in the summer and planned to continue for multiple years. We present here BVOC concentration from the summer and early fall alongside measurements of BVOC oxidation products, ecosystem function, and other relevant atmospheric constituents (e.g. NO_x). We focus here on instrument validation, the relative importance of various compounds and compound classes in the chemical destruction of ozone within the forest canopy, and the formation of regional particulate matter from BVOCs.

2RA.5

Biogenic Oxidation Products in a Mixed Forest: Their Concentrations, Reactivity, and Fates. GRAHAM FRAZIER, Chenyang Bi, Deborah McGlynn, Sally Pusede, Gabriel Isaacman-VanWertz, *Virginia Tech*

Volatile organic compounds emitted from biogenic sources represent the major source of reactive carbon into the atmosphere. Understanding the impacts of changing climate conditions on these emissions is important for predicting future particle and ozone concentration in addition to future climate conditions. In particular, intra- and inter-annual variability of ozone concentrations may impact the emissions of terpenes from vegetation in complex ways that are currently poorly understood by models. We present here early data from a new long-term field deployment to better understand the relationship between regional vegetation emissions, formation of particulate matter, and chemical reactions that change ozone concentrations. Detailed measurements of atmospheric composition were collected in and above a forest canopy in western Virginia representative of forest ecosystems in the southeastern US. This work focuses on understanding the chemical oxidation products of biogenic emissions by molecular characterization of the oxidation products of isoprene, monoterpenes, and sesquiterpenes, alongside measurements of precursor species. We deployed a semi-volatile thermal desorption aerosol gas chromatograph (SV-TAG) to measure the products of biogenic emissions. Particles and semi-volatile gases were collected and analyzed by gas chromatograph/mass spectrometry with hourly time resolution for a one-month period in the summer. We present concentrations of oxidation products and their precursors and discuss them in the context of particle sources, ecosystem function, and the ozone budget. In particular, we examine the extent to which these compounds may represent sources or sinks of oxidants, and what impact that role has on their fate in the environment.

2RA.6

Ultrafine Particle Composition and Growth in the Amazon Basin: Observations from Two Surface Sites. HAYLEY GLICKER, Sarah Batalha, Julio Tota, Alex Guenther, James Smith, *University of California, Irvine*

The Amazon Basin serves as an interesting location to study atmospheric particle formation since it often represents natural, pre-industrial conditions but can also experience periods of anthropogenic influence due to emissions from large agricultural and urban areas. Ultrafine (sub-100 nm diameter) particles are often observed in this region, although new particle formation events seldom occur near the ground despite being readily observed in other forested regions with similar emissions. This study presents measurements of the physical and chemical properties of ultrafine particles and related measurements such as meteorology, bulk particle composition, and key gas phase compounds obtained at two sites in the Amazon Basin: the T3 site from the GoAmazon2014/5 campaign, located 70 km southwest of Manaus, Brazil, and the Tapajós KM67 Mature Forest site located 600 km east of Manaus near Santarém, Brazil. We use these observations to infer possible factors that influence the formation and growth of ultrafine particles in this region. Measurements at the T3 site were performed during the wet season during GoAmazon2014/5, and featured a Thermal Desorption Chemical Ionization Mass Spectrometer (TDCIMS), which measured the concentrations of the most abundant compounds detected in ultrafine particles. Measurements at the KM67 site were performed during the transition between the wet and dry season in 2014 and periodically during a 12-month period in 2016-17, and included size distribution, volatile organic compounds measurements, and ultrafine particle collection followed by offline chemical analysis. The latter was performed using a Sequential Spot Sampler (Aerosol Devices, Inc.) located downstream of a size-selecting nanometer Differential Mobility Analyzer. Comparisons between particle size distributions at each location, supported by air mass back trajectories using the HYSPLIT model, provide insights into the potential influences on particle composition. Each region highlights specific differences in regional chemistry, as anthropogenic influence is seen to a larger extent at the T3 site and agricultural influence is observed more at KM67. The anthropogenic influence at the T3 site is manifested in enhanced levels of particulate sulfate in a background composition consisting largely of organics with significant amounts of nitrogen-containing organic compounds. During times of direct Manaus influence, higher number concentrations of particles over the diameter range of 10-200 nm were observed at T3, while times of background influence had lower number concentrations of these particles with minimal formation and growth events. In contrast, regional ultrafine particle formation and growth events were observed in particles at KM67 during evening hours, starting at particle diameters of ~20 nm with characteristic growth rates of 8 nm/hr. Offline chemical analysis of ultrafine particles collected at KM67 will be compared to TDCIMS measurements performed at T3, and differences relative to the suspected emission sources are discussed.

2RA.8

Comparison of Antarctic and Arctic Seasonal Cycles of Aerosol Chemical Components. LYNN RUSSELL, Amanda Frossard, Patricia Quinn, Sangeeta Sharma, Richard Leitch, Dan Lubin, *Scripps Institution of Oceanography*

In this study, we compare the Antarctic and Arctic seasonal cycle of aerosol chemical components. The distribution of aerosol particles in the Antarctic is characterized by its unique location and surrounding ocean (which largely isolates it from the sources present in other continents), its near-complete coverage by ice and snow (which eliminates most local dust and terrestrial biological particle sources), and its near-absence of human activities (which minimizes the emissions from combustion, cooking, and other human activities). The lack of orographic features in the Southern Ocean surrounding Antarctica supports the midlatitude westerlies, effectively overriding substantial transport of continental emissions into the Antarctic region. The result is that aerosol concentrations reflect the seasonal trends of ocean phytoplankton (sulfate), seabirds (organic), and wind-driven sea spray (salt).

The highest sulfate and organic mass concentrations in the annual cycles in the Arctic at both Barrow and Alert show the well-known springtime haze that results from transport from the northern mid-latitudes. The overall low concentrations of submicron mass concentration are otherwise a common feature of the Arctic and Antarctic. The spring sulfate mass concentrations exceed summer and winter by a factor of more than 2, obscuring the smaller differences between summer and winter seasons. The Barrow and Alert measurements both show higher salt in winter, which likely tracks with winds but could be either from transported sea spray or frost flowers or possibly blowing snow. The prevalence of nearby new sea ice and the depletion of Na relative to Cl are consistent with frost flowers being a main contribution. Another interesting difference is the relative amount of sulfate to organic, which is nearly 1:1 in summer at AWARE and Barrow, but it exceeds 2:1 at Alert, especially in early spring. The higher organic and sulfate mass concentration in summer in Antarctica is coincident with higher concentrations of CCN at supersaturations of 0.1% and 1%. This correlation means that the biogenic sulfate and organic sources may well both contribute significantly to summertime CCN concentrations. The relationship between biogenic sulfate and organic means that both can have an effect on cloud droplet number concentrations, potentially decreasing cloud drop effective radius and shortwave reflection.

2RA.9

Boundary Layer Characteristics and PM_{2.5} Concentration Diurnal Variation on Cloudless Days in Beijing Based on UHF Wind-profiler and Related Meteorological and Air Quality Observations. YUFANG TIAN, Daren LYU, *Institute of Atmospheric Physics, Chinese Academy of Sciences*

Based on boundary layer wind-profiler observations, this study revealed important characteristics of the diurnal variation of atmospheric refractive index structure parameter (Cn₂) on cloudless days in Beijing. By investigating the vertical distribution of Cn₂ on a total of 114 completely cloudless days over a two-year period (March 2011 to March 2013), three patterns of Cn₂ diurnal variation were found. Pattern 1 showed weak diurnal variation, happening in winter months and with low humidity. Pattern 3 showed obvious diurnal variation, with larger Cn₂ at nighttime and smaller values during daytime, detected in high humidity months. In the transition months, with transitional characteristics between patterns 1 and 3, there was Pattern 2. Patterns 1, 2 and 3 accounted for 40.3%, 12.3% and 47.4% of cloudless days, respectively. Variations in characteristics between the three patterns were found to be related to the variation in dominant air flow, terrain effects, and echoing mechanisms. Higher humidity and echoes scattering from anisotropic structures in the refractive index resulted in higher Cn₂.

Since this study covered the characteristics of the whole boundary layer, which provided information on a variety of boundary layer processes, the closely related air pollutant properties in each pattern were also investigated.

PM_{2.5} concentrations were highest in Pattern 1 and lowest in Pattern 3. The concentrations of PM_{2.5} demonstrated diurnal variation for each pattern, with larger values at nighttime, corresponding to the higher humidity at nighttime than during daytime. However, the differences in PM_{2.5} concentrations between nighttime and daytime were largest in Pattern 1 and smallest in Pattern 3. These characteristics were the combined result of the lower atmospheric wind speed, the Cn₂-indicated turbulence intensities in the daytime and the function of higher humidity at nighttime, the inversion layer occurrence rate, and vertical motions.

2RA.10

Chemical and Microphysical Properties of Wind-blown Dust Near an Actively Retreating Glacier in Yukon, Canada. PATRICK HAYES, Jill Bachelder, Malo Bernhard, Carolyn Liu-Kang, Perrine Lambert, Alexane Filoche, Juliana Galhardi, Madjid Hadioui, Marie Cadieux, Amélie Chaput, Marie-Pierre Bastien-Thibault, Kevin Wilkinson, James King, *Université de Montréal*

Airborne mineral aerosols emitted in high-latitude regions can impact radiative forcing, biogeochemical cycling of metals, and local air quality. The impact of dust emissions in these regions on the atmosphere and environment may change rapidly, as warming temperatures can increase mineral dust production and source regions. As there exists little research on mineral dust emissions in high-latitude regions, we have performed the first study of the physico-chemical properties of mineral dust emitted from a sub-Arctic proglacial dust source. Soil and aerosol samples (both PM₁₀ and deposited mineral dust) were collected in May 2018 and 2019 near the Ä'äy Chù (Slims River), a site that has exhibited strong dust emissions. WHO air quality thresholds were exceeded at several receptor sites near the dust source, indicating a negative impact on local air quality. Notably, temporally averaged particle size distributions of PM₁₀ were very fine as compared to those generally measured at low-latitude dust sources. Mineralogy of ambient PM₁₀ comprised primarily clay mineral aggregates, while PM₁₀ elemental composition was enriched in trace elements as compared to deposited dust, bulk soil samples, and the fine soil fraction ($d < 53 \mu\text{m}$). Finally, using analyses of the elemental composition of the soils and of the PM₁₀, of the ambient PM₁₀ particle size distribution, and of meteorological factors measured during our sampling campaign, we propose that the primary mechanisms for dust emissions from the Ä'äy Chù Valley are the rupture of clay coatings on particles and/or the release of resident fine particulate matter.

2RA.11

Aerosol Vertical Distribution Climatology Over India: Dust, Smoke and Polluted Dust. Padmavati Kulkarni, SREEKANTH VAKACHERLA, *CSTEP, India*

Despite several independent observational studies, a comprehensive and climatological picture on the aerosol vertical distribution and its spatial gradients has not yet evolved over the Indian subcontinent. The present study analyses around 10 years of version 3, level 3, Cloud Aerosol Lidar with Orthogonal Polarization (CALIOP) spaceborne lidar (light detection and ranging), retrieved night time, cloud free vertical extinction profiles (at 532 nm) of composite aerosol, and its major species (dust, polluted dust, and smoke), to understand the three-dimensional distribution of aerosols over India.

The shape and vertical extent of the extinction profiles varied in space (from south to north of India) and time (across seasons). Altitudinal decay (decrease with increasing altitude, here and elsewhere) in the aerosol extinction values is steeper over the northern and eastern parts of India, compared to the southern regions of the country. The vertical extent of the aerosol distribution is shallower in the colder seasons compared to warmer seasons, which could potentially be due to suppressed convection during the colder months. Meridional gradients have been observed in the surface extinction coefficients. Polluted dust, which can be defined as a mixture of dust and smoke, emerged as the dominant aerosol species over most parts of the study region.

Over the north-western and central India, dust aerosols contributed the most to aerosol optical depths and extinction profiles, during the summer and monsoon months. Smoke aerosols, which have been attributed to biomass, agricultural burning, and long-range transport, prevailed over the southern and north-eastern regions of India. Boundary layer aerosol optical depths (AOD) contributed to columnar AOD significantly during the post-monsoon and winter seasons. Meanwhile the elevated AOD has an equal share in columnar AOD during the summer and monsoon seasons.

2RA.12

Characterizing Primary Ultrafine Particle Sources in the United States with CMAQ-UF. BENJAMIN MURPHY, Francis Binkowski, Ekbordin Winijkul, Matthew Alvarado, *United States Environmental Protection Agency*

We have updated the Community Multiscale Air Quality (CMAQ) model v5.3 with new algorithms and data to represent the emission, secondary formation, and growth of ultrafine particles. This enhanced model, CMAQ-UF, is evaluated with measurements from several urban and rural sites throughout the US. We then analyze CMAQ results at the continental US level to determine the sensitivity of ultrafine particle exposure to important model parameters governing both primary and secondary introduction of new particles.

We have shown previously that organic compounds and amines can participate with sulfuric acid to form new particles or, when sulfuric acid concentrations are low, generating particles on their own. These processes are an important regional driver of ultrafine particle concentrations whereas primary emissions are the fundamental source for ultrafine particles in urban and industrialized areas. We have incorporated our robust algorithm for new particle formation and growth along with state-of-the-science parameterizations of the size distribution of primary particle emissions from more than 40 source classes (e.g. vehicles, natural gas operations, coal-fired power plants, wildfires, etc.) into a detailed annual simulation of ultrafine particle sources and fate in the United States.

We apply the new model to observations made throughout the US including California (the CalNex and CARES 2010 campaigns), and the Denver DISCOVER-AQ campaign. The qualities of these and other observation sites allow us to constrain the model in urban, suburban, and rural locations, which is critical since the drivers of ultrafine particle concentrations are expected to change dramatically among these receptor types. Characterization of ultrafine particle pollution with CMAQ-UF improves our understanding of the most effective ways to mitigate the highest concentrations in the US.

2SA.1

Impacts of Household Sources on Air Pollution at Village and Regional Scales in India. BRIGITTE ROONEY, Ran Zhao, Yuan Wang, Kelvin Bates, Ajay Pillarisetti, Sumit Sharma, Seema Kundu, Tami Bond, Nicholas Lam, Bora Ozaltun, Li Xu, Varun Goel, Lauren Fleming, Robert Weltman, Simone Meinardi, Donald Blake, Sergey Nizkorodov, Rufus Edwards, Ankit Yadav, Narendra Arora, Kirk Smith, John Seinfeld, *California Institute of Technology*

Approximately 3 billion people worldwide cook with solid fuels such as wood, charcoal, and agricultural residues. These fuels are often combusted in inefficient devices, producing carbonaceous emissions. More than 2.6 million premature deaths occur as a result of exposure to fine particulate matter from the resulting household air pollution. Household air pollution also contributes to ambient air pollution; however, the magnitude of this contribution is uncertain. We simulate the distribution of a major health-damaging outdoor air pollutant, PM_{2.5}, using state-of-the-science emissions databases and atmospheric chemical transport models to estimate the impact of household combustion on ambient air quality in northern India. We employ an emissions inventory prepared based on a national inventory in India, an updated residential sector inventory, updated cookstove gas emissions factors from field studies, and PM_{2.5} speciation from cooking fire experiments. We simulate regional air quality using the U.S. Environmental Protection Agency Community Multiscale Air Quality modeling system (CMAQ), in conjunction with the Weather Research and Forecasting modeling system (WRF) to simulate meteorological inputs for CMAQ and the global chemical transport model GEOS-Chem to generate boundary conditions of the computational domain. Comparisons between observed and simulated PM_{2.5} levels during September 2015, December 2015, and September 2016 at urban and rural sites in northern India are carried out to assess overall airborne levels and to estimate the contribution of household cooking emissions. Residential emissions are predicted to account for about 10% and 27% of anthropogenic PM_{2.5} in New Delhi and at rural sites, respectively. Of PM_{2.5} produced by household combustion, up to 80% is predicted to be secondary organic matter (SOA) during September months. Predicted levels of total SOA averaged about 30 μg m⁻³, representing approximately 30% and 20% of total PM_{2.5} levels in rural and urban areas, respectively.

2SA.2

Source Attribution Using Fourier Transform Infrared Spectroscopy in the Interagency Monitoring of Protected Visual Environments (IMPROVE) Network. ANDREW WEAKLEY, Alexandra Boris, Bruno Debus, Satoshi Takahama, Ann Dillner, *University of California, Davis*

Ambient fine aerosols describe sub-micron condensed phase compounds (<2.5μm particle diameter) derived from primary emission sources (e.g., motor vehicle exhaust) and secondary gas-to-particle formation mechanisms in the atmosphere. Presently, only a fraction of the species comprising ambient fine aerosols are identified and quantified given limited theoretical knowledge of aerosol composition and consequent unavailability of standards. Fourier transform infrared (FT-IR) spectra have successfully probed functional group (FG) composition when applied to filter-bound fine aerosol samples collected from several US monitoring networks. As such, cluster analysis algorithms applied to FT-IR spectra may prove useful in attributing FG absorption to particular sources and/or understanding regio-temporal fluctuations in fine aerosol composition at the functional group level. To this end, a Gaussian Mixture Model (GMM) was fitted to approximately 20,000 Interagency Monitoring of PROtected Visual Environments (IMPROVE; 2015 sampling year) spectra following derivative transformation (to suppress baseline in the spectra), spectra normalization (to emphasize relative FG absorption), and a principal component analysis (to reduce dimensions of input data). Source-cluster assignments were accorded to changes in species-specific FT-IR absorption bands and supported by deviations from concentration normalized median fine carbon (i.e., OC and EC), nitrate and sulfate, and element (e.g., Si, Na) mass concentrations. Most clusters exhibited moderate-to-strong association between region (e.g., eastern US) and season including Midwest samples with elevated inorganic nitrate absorption (winter dominant), southwest samples distinguished by silica IR absorption attributable to African dust storms (spring dominant), eastern US samples showing elevated inorganic sulfate mass (summer), and wildfire samples collected from the northwest (summer). Other clusters, exhibiting less regional or temporal association, included samples impacted by marine aerosol as well as those connected to volcanic activity (AK and HI). Overall, FT-IR spectroscopy appears as a valuable tool for non-destructive aerosol source attribution.

2SA.3**Elucidating Sources and Human Health Risk of Inhalation Exposure to VOCs and PM_{2.5} at Albany, New York.** MD.AYNUL BARI, Sanchita Paul, *University at Albany, SUNY*

Exposure to ambient VOCs and PM_{2.5} in urban areas is of interest because of their potential adverse effects to public health. A study was carried out to better elucidate ambient sources of VOCs and PM_{2.5} in Albany, the Capital of New York State for the period 2015–2018. Twenty-four hour average concentrations of measured total VOCs and PM_{2.5} were low – 5.4 µg/m³ (range: 1.8–12.4 µg/m³) and 6.4 µg/m³ (0.5–22.6 µg/m³), respectively. A combined dataset of VOCs and PM_{2.5} species was used in positive matrix factorization (PMF) model to better interpret the complex nature of different sources. Ten sources were revealed where secondary organic aerosol (SOA) (1.8 µg/m³, 33%) and diesel vehicles/global background (1.0 µg/m³, 19%) were the largest contributors to VOCs. Predominant contributors to PM_{2.5} were SOA (1.1 µg/m³, 18%) and spark-ignition (gasoline) (1.1 µg/m³, 18%) followed by secondary sulfate (0.9 µg/m³, 14%), secondary nitrate (0.7 µg/m³, 11%) and diesel vehicles (0.6 µg/m³, 10%). Other sources included combustion-related, vehicle exhaust, road-salt, soil dust, and methyl ethyl ketone-rich. Source-specific carcinogenic and non-carcinogenic health risk values were also calculated. Estimated carcinogenic risks for all sources were below the U.S.EPA acceptable level except for SOA and diesel vehicles/global background, where they posed greater risk to public health (48% and 14% of carcinogenic risk, respectively) compared to other sources. Due to lack of some VOC species data (e.g., alkanes, alkenes), other urban sources e.g., petroleum-related and fuel evaporation were not identified. More work is needed to understand the origin of potential SOA and wintertime biomass combustion sources in Albany county and surrounding region. Findings of this study can support policy makers in developing appropriate air quality management initiatives if needed.

2SA.4**Using Highly Time-resolved Data to Improve the Lake Michigan Ozone Study: Particle Size Distributions and VOCs at a Coastal Site.**MEGAN CHRISTIANSEN, Austin Doak, Dagen Hughes, Charles Stanier, Elizabeth Stone, Dylan Millet, Hari Prasad Alwe, *University of Iowa*

The collaborative field campaign, Lake Michigan Ozone Study 2017, occurred between May 22–June 22, 2017. The campaign combined ground site, mobile, aircraft, and ship measurements to better understand the ozone episodes around Lake Michigan. Particle size distributions (PSD) were measured at the main ground site (Zion, IL) with a Scanning Mobility Particle Sizer (SMPS) and Aerodynamic Particle Sizer (APS) and volatile organic compounds (VOCs) with a proton-transfer-reaction mass spectrometer (PTR-MS). The high time resolution of these data allows for the source receptor modeling to resolve local sources that periodically impact the site.

The Zion site is influenced by several local sources of air pollution within 1 km: traffic and cooking in the state park, commuter rail, and an arterial roadway. Transport to the site is heavily influenced by a lake breeze flow from Lake Michigan during early summer, especially on days with ozone above 70 ppb. PM_{2.5} mass reconstructed from the PSD compared favorably with collocated gravimetric filters (5.06 vs. 6.81 µgm⁻³). The average number concentration from 3 nm – 10 µm was 8258 cm⁻³ and from 3 – 10 nm was 1108 cm⁻³. Particle number and mass were positively correlated with ozone and its precursors. Preliminary Positive Matrix Factorization (PMF) identifies a nighttime aromatic hydrocarbon factor to the west, an acetonitrile rich factor from the southwest, and several other factors. Preliminary PMF of PSD show nuclei mode in the lake breeze and several other directionally specific ultrafine factors.

Diel patterns and wind direction dependence will be used to locate nearby sources, while potential source contribution functions (PSCF) and Concentration Weighted Trajectory (CWT) will be used to locate sources within the University of Iowa 4x4 km LMOS 2017 WRF-Chem modeling grid. PSCF uses hourly back trajectories processed in HYSPLIT to locate probable source grid cells.

2SA.5**Source Apportionment and Temporal Trends of Coarse Particulate Matter (PM): A Case Study in Central Tehran, Iran.**

EHSAN SOLEIMANIAN, Sina Taghvaei, Amirhosein Mousavi, Mohammad Sowlat, Mohammad Sadegh Hassanvand, Masud Yunesian, Kazem Naddafi, Constantinos Sioutas, *University of Southern California*

Positive matrix factorization (PMF) receptor model was employed to identify the sources of coarse particulate matter (PM) and their corresponding seasonal variations in two locations (i.e., a school dormitory and a retirement home) in central Tehran. Daily samples were collected from ambient PM using low-volume air samplers (FRM OMNUTM air sampler, multi-cut inlet; BGI, USA) within May 2012 to June 2013. Water-soluble ions, metals, and trace elements were used as the input data to the PMF model after analyzing the chemical constituents of the filter samples. Results represented an annual coarse PM average concentration of $45.7 \pm 3.8 \mu\text{g}/\text{m}^3$ and $38.4 \pm 4.5 \mu\text{g}/\text{m}^3$ at the school dormitory and the retirement home, respectively, with higher concentration in summer as opposed to the winter phase. PMF solutions suggested road dust, soil and industry, and sea salt as the three major sources of ambient coarse PM in central Tehran with the corresponding contributions of $74 \pm 9\%$, $19 \pm 2\%$, and $7 \pm 1\%$ to total coarse PM mass concentration, respectively. The temporal trends of the resolved factors indicated higher contribution of road dust to total coarse PM mass concentration during warm phase as a result of higher wind speed and temperature as well as lower relative humidity which leads to an increase in resuspension rate from road surfaces. Additionally, dust storms in combination with higher resuspension rate of mechanically originated particulates led to higher summertime contribution of soil factor to coarse PM. Results from this study provide insight regarding the importance of non-tail pipe emissions on ambient coarse PM mass concentration in Tehran.

2SA.6**Application of Advanced Factorization Techniques for Deconvolution of Cooking and Biomass Burning Source Contributions in a Polluted Megacity.** SAHIL BHANDARI, Kanan Patel, Shahzad Gani, Gazala Habib, Joshua Apte, Lea Hildebrandt Ruiz, *University of Texas at Austin*

Application of receptor modeling techniques to data from online mass spectrometers has provided insight into the nature and sources of atmospheric aerosol. Positive matrix factorization (PMF) is one such technique which deconvolutes sampled data into the summation of products of positively constrained mass spectral profiles and their corresponding time series, under the assumption that the mass spectral profiles remain constant in time. However, application of PMF to unit mass spectral (UMR) data often does not resolve primary organic aerosol (POA) to hydrocarbon-like organic aerosol (HOA), cooking organic aerosol (COA), and biomass burning organic aerosol (BBOA), even in highly polluted environments. To address this issue, we applied advanced factorization techniques including time-resolved PMF and ME-2 (a hybrid of Chemical Mass Balance (CMB) technique and PMF using a priori information of factor profiles to constrain their presence) to data collected in the Delhi Aerosol Supersite (DAS) study.

For example, applying these techniques to the evenings of winter 2017 separates HOA, oxidized organic aerosol (OOA), BBOA, and oxidized biomass burning organic aerosol (OBOA), compared to two-factor solutions in seasonal PMF runs (HOA and OOA). Also, a narrowing time window around afternoon cooking hours results in increasing fresh COA signatures in the POA profile.

Overall, these techniques enable the generation of multiple sets of factor profiles over diurnal time windows in each season. Profiles obtained using these methods, therefore, offer a more realistic picture of temporally varying sources and the evolving oxidized organic aerosol.

2SA.7**Spatial Variation of Wintertime Aerosol Composition and Source Contribution across the Kathmandu Valley, Nepal.**

BENJAMIN WERDEN, Michael Giordano, Khadak Mahata, Siva Praveen Puppala, Arnico Panday, Robert J. Yokelson, Elizabeth Stone, Peter DeCarlo, *Drexel University*

The Nepal Ambient Monitoring and Source Testing Experiment [NAMaSTE 2] in December 2017- February 2018 measured aerosol composition and source apportionment across the Kathmandu Valley, Nepal. Ambient measurements were made at three locations from urban, to suburban, and the rural valley edge.

The urban site, Ratnapark, was heavily impacted by traffic, and the observed average PM_{10} concentration was $74 \pm 39.6 \mu g \cdot m^{-3}$, consisting of 41% organics, 7% sulfate, 35% BC, 5% ammonium, 6% nitrate, and 5% chloride. The suburban site, Lalitpur, was subject to emissions from brick kilns; the average PM_{10} was $79.63 \pm 38.7 \mu g \cdot m^{-3}$, consisting of 44% organics, 11% sulfate, 26% BC, 7% ammonium, 8% nitrate, and 4% chloride. Dhulikhel, at the valley edge, had minimal influence from industry, and the average PM_{10} was $35.42 \pm 14.4 \mu g \cdot m^{-3}$, consisting of 56% organics, 8% sulfate, 17% BC, 6% ammonium, 10% nitrate, and 2% chloride.

Positive Matrix Factorization identified several distinct factors for the organic mass spectra measured. Commonly observed Organic Aerosol (OA) factors identified were, Hydrocarbon (HOA), Cooking (COA), Coal Combustion (CCOA), Biomass Burning (BBOA), and both semi- and low-volatile oxygenated OA (SV-OOA, LV-OOA). HOA increased at all sites during rush hours, as did COA during meal times. LV-OOA was a consistently observed background aerosol in the valley. Overnight increases of CCOA and sulfates were seen and BBOA concentrations increased substantially overnight. Trash burning was a significant factor in the urban environment.

Differences in source concentration at each measurement location is important to document so that effective mitigation measures can be designed appropriately across the region.

2SA.8**Source Apportionment of Multiple Metals in PM_{2.5} in Beijing, China.** MEI ZHENG, Xi Yang, Junyi Liu, *Peking University*

Sources of multiple metals in PM_{2.5} including K, Ca, Fe, Zn, Pb, Ba, Mn, Cu, As, Se, Cr, and Ni were investigated in this study, which were measured for one year at 1-h resolution in Beijing by a Xact TM625 multi-metal monitor (from September 2016 to July 2017) at an urban site in Beijing. The levels of atmospheric metals in Beijing are lower than some other industrial cities in China, but two or three orders of magnitude higher than some cities in Europe and the U.S. They exhibited clear seasonal variations, with higher concentration in winter than summer. The comparison between haze and non-haze periods for metals was made to examine sources that contribute to the increase of fine particles during haze periods. In addition, positive matrix factorization (PMF) was applied for source apportionment of metals in PM_{2.5}, and four factors including industry, vehicular exhaust, dust, and coal combustion were identified and quantified. The relative importance of different sources varied from metal to metal. The trajectory analysis indicated that the transport from the south of Beijing could contribute to some high level of metals during episodic events.

2SA.9

Insights into PM_{2.5} 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*

Serious haze events in Beijing are mostly characterised by fine particulate matter (PM_{2.5}) and extreme pollution events are dominated by secondary aerosol (Huang *et al.*, 2014). The recent development of a novel extractive electrospray ionisation long-time-of-flight mass spectrometer (EESI-LTOF, Lopez-Hilfiker *et al.*, 2019) enables rapid, online OA measurements at atmospherically relevant concentrations with soft ionisation, providing near-molecular chemical information while avoiding thermal decomposition or ionisation-induced fragmentation, which potentially enable the identification and quantification of secondary organic aerosols.

As the first trial of field-deployable EESI-LTOF implementation in heavy mass loading condition, an intensive online campaign in Beijing was conducted from the beginning of October to mid-December using an EESI-LTOF, together with an Aerodyne long-time-of-flight aerosol mass spectrometer (L-TOF-AMS) equipped with a PM_{2.5} aerodynamic lens and other supporting measurements. OA sources/processes were investigated by positive matrix factorisation (PMF) implemented by the multilinear engine (ME-2) using the Source Finder (SoFi) interface (Canonaco *et al.*, 2013).

This ten-week campaign covers two distinctive periods: autumn non-heating season and winter heating season. PMF analysis of AMS resolves four primary sources (cooking-related OA, coal combustions OA, biomass burning OA and hydrocarbon-like OA) and four secondary factors (two less oxygenated OAs and two more oxygenated OAs). Among the eight factors, SOA accounts for a significant and sometimes dominant fraction of OA, highlighting the importance of determining the physicochemical and/or meteorological processes governing SOA accumulation. Interestingly, one less oxygenated OA and one more oxygenated OA contribute more mass in the non-heating season haze events than heating season haze, whereas the other less oxygenated OA shows the opposite pattern. The limited chemical information provided by the AMS makes a mechanistic interpretation challenging, and we exploit EESI-TOF tracer ions and PMF analysis to constrain the sources and physicochemical processes governing SOA accumulation during extreme haze.

2SA.10

Source Apportionment of Submicron Aerosol Particles in a Mediterranean Harbour by Using a Rolling Window Approach. BENJAMIN CHAZEAU, Grégory Gille, Boualem Mesbah, Brice Temime-Roussel, Francesco Canonaco, Andre S.H. Prévôt, Barbara D'Anna, Henri Wortham, Nicolas Marchand, *Aix-Marseille Université, CNRS, LCE FRE 3416*

Marseille is the largest harbour of the Mediterranean Sea and is a challenging environment for air quality. 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-Longchamp (MRS-LCP).

A real-time dataset collected between February 2017 and August 2018 is presented here. ToF-ACSM organic aerosol (OA) mass spectra were analyzed by means of Positive Matrix Factorization (PMF) using the multilinear engine (ME-2) approach. 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.

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) is the dominant aerosol source during winter, mainly advected 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 but the most interesting feature regards the submicron particles number concentration and their size distribution. Very intense plumes (N_{tot}>80 000 cm⁻³) associated with SO₂ and metals are observed systematically when sea breezes bring back over the city air masses impacted by industrial and shipping emissions.

2SA.11

High Time Resolution Observation and Its Source Apportionment of Brown Carbon during Winter and Summer in Urban Xi'an, Northwestern China. YALI LEI, Zhenxing Shen, Tian Zhang, DI LU, Yaling Zeng, Qian Zhang, Hongmei Xu, Jianhuai Ye, Yiming Qin, Xin Wang, Junji Cao, *Xi'an Jiaotong University*

There is a growing evidence suggesting that an enhancement of brown carbon (BrC) in the severe haze episodes. In this study, hourly measurements of BrC in $PM_{2.5}$ were conducted in Xi'an, a typical city in Northwestern China, during the winter (1 January to 6 January) and the summer (24 July to 5 August) of 2017. Filters were extracted in methanol. The light-absorbing properties of the solution were quantified using UV-vis spectroscopy. Results showed that the absorption coefficient at 365 nm ($b_{365, \text{methanol}}$) in winter was over 7 times higher than that in summer, while the mass absorption cross-section ($MAC_{365, \text{methanol}}$) in winter for BrC was nearly double of that in summer. During the winter haze days, the average $b_{365, \text{methanol}}$ peaked at 00:00 am LT with the lowest values observed at 7:00 am LT in the morning, contrary to the high afternoon and low nighttime levels observed in non-haze days. Unlike the diurnal patterns in winter, average summer $b_{abs365, \text{methanol}}$ diurnal variation presented high mid-day and low afternoon levels in haze days. However, in non haze days, the pattern showed morning high levels and night low levels. Source apportionment of $b_{abs365, \text{methanol}}$ based on the positive matrix factorization receptor model and multiple linear regressions showed the $b_{abs365, \text{methanol}}$ of secondary formation accounted for 28.0 % (winter) and 74.5 % (summer) of total $b_{abs365, \text{methanol}}$, indicating that secondary formation was an important contributor to BrC emissions over Xi'an during both winter and summer.

2SA.12

High Time-Resolution Measurements of Ambient Metals and Elements in Los Angeles: Source Apportionment and Temporal Variations. SINA HASHEMINASSAB, Payam Pakbin, Andrea Polidori, Aaron Katzenstein, Jason Low, *South Coast Air Quality Management District*

The Los Angeles Basin is home to some communities that encompass several metal-processing facilities in close proximity to each other and to residential neighborhoods. In 2016, the South Coast Air Quality Management District initiated an extensive investigative air monitoring campaign to identify and address sources of hexavalent chromium (Cr6+) and other toxic metals in the City of Paramount. Using portable air samplers, 24-hr time-integrated filter samples were collected every third day at a total of 48 different locations throughout the City for toxic metals analysis. Highly elevated levels of Cr6+ were found initially and additional efforts were conducted to better characterize sources of Cr6+ and other metals that were be impacting nearby communities. As part of these efforts, hourly concentrations of several metals were measured continuously with Xact 625 (Cooper Environmental Services, OR, USA) at two locations. This air monitoring campaign has been ongoing since 2016.

Air monitoring results indicated a substantial reduction in ambient levels of Cr6+ over time. This was achieved through rule amendments, enforcement actions, and voluntary emissions mitigation. Xact measurements provided useful information on the temporal trends of metals including their diurnal, day-of-week, and seasonal variations. The high time-resolution measurements also enabled investigating the impact of exceptional events (e.g., 4th of July fireworks) on the levels of ambient metals. A Positive Matrix Factorization (PMF) source apportionment model on the Xact data identified four source categories (i.e. soil/road dust, industrial emissions, vehicular abrasion, and residential wood smoke) with distinct profiles and temporal variations. Moreover, Conditional Probability Functions (CPFs) were computed using hourly wind data for individual species and PMF-derived source categories to identify the local source directions.

2UA.1**Integration of Ground-Based Particulate Matter Measurements with Satellite Observations in the Multi-Angle Imager for Aerosols (MAIA) Investigation.**

SINA HASHEMINASSAB, Kristal Verhulst, Michael Garay, Abigail Nastan, Randall V. Martin, Yang Liu, David Diner, *Jet Propulsion Laboratory*

NASA's upcoming Multi-Angle Imager for Aerosols (MAIA) investigation (expected launch in 2022) is designed to study the adverse health effects of exposure to ambient particulate matter (PM) and its major chemical constituents. Observations collected by the MAIA satellite instrument, currently being built at JPL, will be matched with ground-based PM measurements in order to generate geostatistical regression relationships that will enable mapping of PM_{2.5} and PM₁₀ total mass and speciated PM_{2.5} (sulfate, nitrate, ammonium, organic carbon, black carbon, and dust) at 1-km spatial resolution. This process will be carried out within a selected set of highly populated metropolitan areas distributed around the world. The resulting data products will be used by epidemiologists on the team and their collaborators to study acute, sub-chronic, and chronic health effects of PM having different proportions of size and compositional components.

Generation of the MAIA data products relies on the availability of sufficient ground-based PM monitors to relate aerosol properties measured from space to the PM levels on the ground. In this presentation, we will provide an overview of the MAIA investigation and discuss our progress in identifying and accessing existing ground-based PM data provided by governments, research groups, and other sources in the selected target areas. We will also discuss our efforts to evaluate and deploy additional monitors for PM total mass and species measurements in order to ensure adequate representation of surface measurements in the MAIA data processing approach.

2UA.2**Detecting Biomass Burning Using Intensive Aerosol Optical Properties in El Paso, Texas - (BC)2 El Paso Field Campaign.**

SUJAN SHRESTHA, Meghan C. Guagenti, James Flynn, Sergio Alvarez, Sascha Usenko, Rebecca J. Sheesley, *Baylor University*

Emissions from anthropogenic sources (e.g. motor vehicle exhaust and coal-fired power plants) have been significantly reduced in the US through the implementation of cleaner technologies, refocusing our efforts to understand the contribution and impact of biomass burning to urban air quality. This is particularly relevant for El Paso where transport of regional biomass burning can drive plumes into the city from across state and international boundaries, resulting in periodic increases in atmospheric pollutants. To study this phenomenon, the Black and Brown Carbon study or (BC)2 El Paso is conducting field measurements from mid-March through September 2019. For (BC)2, the Baylor air quality trailer has been equipped with two tricolour absorption photometers (TAP), a seven-channel aethalometer (AE42), a three-wavelength nephelometer, and carbon monoxide (CO) and nitrogen oxide (NO_x) analyzers. This study uses intensive aerosol optical properties: Absorption and Scattering Ångström Exponents (AAE and SAE) and Single Scattering Albedo (SSA) along with BC/CO and CO/NO_x ratios to characterize aerosol optical properties in El Paso and to identify biomass burning plumes. SSA, which is the ratio of scattering to total extinction, will determine the net sign of an aerosol's radiative forcing for El Paso under conditions of routine urban emissions and biomass burning events. The simultaneous operation of the TAP and aethalometer provides an opportunity for inter-comparison. Preliminary results indicate an AAE value near 1, which is indicative of motor vehicle exhaust with little influence from biomass burning plumes with higher AAE. Detailed results from the long-term measurements with supplemental HYSPLIT back trajectory analysis and MODIS fire identification products will be presented during the conference.

2UA.3

Identification of the Major Sources of the Particulate Nitrosamines and Nitramines in the Ambient Atmosphere at Seoul, South Korea. NA RAE CHOI, Yun Gyong Ahn, Ji Yi Lee, Yong Pyo Kim, *Ewha Womans University*

Nitrosamines and nitramines are the groups of chemical compounds with the general structure containing nitroso (N-NO) and nitro (N=O) functional group, respectively, and they have been suspected as carcinogens. Nitrosamines and nitramines in the atmosphere can be emitted from the primary emission sources such as industrial use, vehicular exhaust, and other processes like tobacco smoking or cooking. They can be also generated from atmospheric reactions of organic amines and removed by photolysis and oxidation. Simultaneous analysis of nitrosamines and nitramines is necessary to understand the major sources of nitrosamines and nitramines in the ambient atmosphere, since their primary emission sources and atmospheric reactions pathways are related.

Simultaneous analysis of 7 nitrosamines (nitroso dimethylamine, nitroso diethylamine, nitroso dipropylamine, nitroso dibutylamine, nitroso morpholine, nitroso piperidine and nitroso pyrrolidine) and 3 nitramines (methyl nitramine, dimethylnitramine and diethylnitramine) in the atmospheric particulate matter with an aerodynamic diameter of less than or equal to a nominal 2.5 μm (PM_{2.5}) at Seoul for a year (2018.01~2018.12) was carried out by using gas chromatography/tandem mass spectrometry (GC/MS-MS). The annual average concentrations of nitrosamines and nitramines were $10.52 \pm 18.98 \text{ ng/m}^3$ and $1.20 \pm 0.65 \text{ ng/m}^3$, respectively. The seasonal average concentrations of nitrosamines showed the highest concentrations in fall ($18.91 \pm 28.47 \text{ ng/m}^3$) and the lowest concentrations in summer ($2.81 \pm 5.86 \text{ ng/m}^3$). The levels of nitramines showed a different trend, the highest concentrations in summer ($1.79 \pm 0.48 \text{ ng/m}^3$) and lowest concentrations in winter ($0.75 \pm 0.52 \text{ ng/m}^3$). Major sources of the observed nitrosamines and nitramines are to be investigated using the correlation, multivariate analysis and simple kinetic approach based on the ambient concentrations of nitrosamines, nitramines, other organic and inorganic compounds and meteorological parameters which were simultaneously measured.

2UA.4

Effects of Climate and Emission Changes on Air Pollution in India. HAO GUO, Kaiyu Chen, Sri Kota, Hongliang Zhang, *Louisiana State University*

With the rapid growth of industries and population in India, increase of air pollutants emissions is expected and will result in higher pollution levels in future than nowadays without proper control measurements in addition to climate change. This study will investigate the effects of emission and climate change on concentrations of ozone and particulate matter (PM) in India, 2050 using the Community Multi-scale Air Quality (CMAQ) model. The current meteorology will be generated using Weather Research and Forecasting (WRF) model version 3.7.1 and the future meteorology will be generated using the same model under the Representative Concentration Pathways (RCP) 4.5, 6.0 and 8.5 emission scenario. The three future emission scenarios will be developed based on Emissions Database for Global Atmospheric Research (EDGAR) version 4.3 as following: no change case will directly use 2015 emissions for 2050, business as usual (BAU) case will use adjusted emissions in 2050 with proper factors to reflect the growth of industry and population, and controlled case will be based on potential control strategies. The differences in spatial and temporal variations of air pollutants between 2015 and 2050 will be analyzed and the contributions of emission change and climate change in three scenarios will be quantified.

2UA.5

Investigation of the Driving Forces for the Recent Trends in Surface Fine Particulate Matter Concentrations in Nanjing, China. JIANLIN HU, Zhihao Shi, Jingyi Li, Hongliang Zhang, Qi Ying, *Nanjing University of Information Science & Technology*

Meteorological conditions and emissions play very important roles in the formation of PM_{2.5} pollution. PM_{2.5} concentrations in Nanjing have been decreasing rapidly from ~70 µg/m³ in 2013 to ~50 µg/m³ in 2016. The contributions of inter-annual variation of meteorological conditions and emissions to the rapid PM_{2.5} reduction remain unknown. In this study, we used several methods to quantify the contributions. First, we established a generalized linear regression model (GLM) based on meteorological parameters to assess the effect of meteorological conditions and pollution control strategies on reducing the air pollution level in Nanjing. Second, we conducted sensitivity simulations with the WRF/CAMQ model, in which we perturb seven major meteorological parameters, i.e., wind speed, wind direction, temperature, humidity, boundary layer height, precipitation, and cloud cover, and then simulate the changes of PM_{2.5} concentrations to analyze its sensitivity to meteorological variations. Third, we simulated PM_{2.5} concentrations in Nanjing in 2013 and 2015 using different years of emissions to investigate the impacts of emissions change and meteorological variations on PM_{2.5} concentrations. The results using the three methods will be compared and discussed.

2UA.6

Simulation of Heterogeneous Chemistry of SO₂ and NO_x on Mineral Dust Particles in Ambient Environments Using CAMx. ZECHEN YU, Myoseon Jang, *University of Florida*

The surface of mineral dust particles can act as an important sink for atmospheric tracers (e.g., O₃, SO₂, and NO_x) and photochemically enhance the production of oxygenated compounds. During a typical dust event, the extremely high concentration of airborne mineral dust particles is introduced into atmosphere. These dust particles can undergo long-range transport and impact on urban atmospheric environments. However the effects of mineral dust particles on heterogeneous chemistry of inorganic pollutants, such as SO₂ and NO_x are not well studied due to the lack of kinetic mechanisms. Using the Atmospheric Mineral Aerosol Reaction (AMAR) model, our research team recently launched to the simulation of heterogeneous photooxidation of SO₂ and NO_x in the presence of mineral dust particles. The prototype AMAR model was evaluated for the formation of sulfate and nitrate using outdoor smog chamber data under the ambient sunlight. In this work, the AMAR model is extended to regional simulation using the Comprehensive Air Quality Model with Extensions (CAMx) by capturing the heterogeneous formation of sulfate and nitrate during the dust event in urban atmosphere. The simulation results using CAMx-AMAR enable the estimation of the lifetime of inorganic trace gases during the dust event. Furthermore, heterogeneous chemistry of SO₂ and NO_x impacts on the dust's hygroscopicity, which influences the indirect effects of dust particles by the modulation of Cloud Condensation Nuclei activities. The change of hygroscopicity of dust particles also impacts on heterogeneous chemistry of other polar inorganic trace gases, such as N₂O₅ and HONO, as well as the formation of secondary organic aerosols.

2UA.7

Simulation of Evolving Gas- and Aerosol-Phase Air Quality over Los Angeles. ELYSE PENNINGTON, Melissa Venecek, Yuan Wang, John Seinfeld, *California Institute of Technology*

Secondary organic aerosol (SOA) is an important component of urban aerosol, but modeling its mass and speciation remains a challenge. The Community Multiscale Air Quality (CMAQ) model developed by EPA has been widely used to simulate atmospheric chemistry, SOA formation, and responses to changes in emissions. Emissions inventories, a crucial input to CMAQ, for Los Angeles and other regions, are continuing to evolve. For example, McDonald et al. (2018) showed that urban mobile source emissions are declining, while those of volatile chemical products (VCPs) are becoming increasingly important. The 2018 emissions inventory of McDonald et al. over the Los Angeles Basin is incorporated into CMAQ version 5.2. The impact of these changes on CMAQ predictions of gas-phase species and SOA mass and speciation are examined in light of observational data. Prediction of gas-phase and SOA levels and speciation corresponding to the estimated 2018 emissions inventory for Los Angeles is presented. The influence of meteorological fields on the simulated SOA is explored.

2UA.8

Local and Cross-Regional Contributions of Air Quality Policy in Central Taiwan. MIN-CHUAN HSIAO, Hsin-Chih Lai, Wen-Yinn Lin, Joshua S. Fu, Lei-Wei Lai, *National Taipei University of Technology*

Air pollution has become a global issue getting more public concern. Such a small island with a well-developed industry and heavy ongoing traffic like Taiwan, public attention on air quality is increasing even its air quality has been constantly improving since the last decade. To attain the national regulatory goal ($15 \mu\text{g}/\text{m}^3$ for, annual average), counties in Taiwan are currently developing a series of action plan for $\text{PM}_{2.5}$ emission reduction. However, considering the current air quality policies and strategies, it's not easy to meet the national regulatory goal ($15 \mu\text{g}/\text{m}^3$, annual average) in most of the geographical areas in the near future.

The purpose of this study was mainly investigating the contribution of emissions from each county to itself as well as to other counties in central Taiwan and discussing the necessity of cross-region policies by the using the Weather Research and Forecasting (WRF) model and the Community Multiscale Air Quality (CMAQ) model. This study could help understanding the impact proportion of $\text{PM}_{2.5}$ emitted from point, traffic and non-point sources to the air quality. The findings of this research not only offer important insights about the air quality impacts of each country, but also provide useful information for the decision making of cross-regional policy.

2UA.9**Comparison of Chemical Characteristics of PM_{2.5} during Winter Haze Events in Beijing, China and Gwangju, Korea.**

MINHAN PARK, Jihyo Chong, Haebum Lee, Nohhyeon Kwak, Hyunok Maeng, Kyungjoo Kim, Eunbi Lee, Enrique Cosep, A Young Choi, Hangyul Song, Ma. Cristine Faye Denna, Dahye Oh, Min-Suk Bae, Kyoung-Soon Jang, Min Hu, Xiaoyang Yang, Kihong Park, *Gwangju Institute of Science and Technology*

Particulate matter less than 2.5 μm (PM_{2.5}) in the ambient atmosphere is of great interest due to its effects on human health and climate change via radiation balance and cloud formation. Simultaneous measurements of chemical characteristics (ions, elements, elemental carbon, organic carbon, organic compounds, and Pb isotopes) of PM_{2.5} were conducted during wintertime (1/3/2018-2/2/2018) at urban sites (Beijing, China and Gwangju, Korea). Filter samples were collected daily for offline measurements such as ions, organic carbon (OC), elemental carbon (EC) and elements as well as organic compounds and Pb isotopes at both sites. The average mass concentration of PM_{2.5} at Beijing was much higher than those at other sites; Beijing (62.45 \pm 34.09 $\mu\text{g}/\text{m}^3$) and Gwangju (26.77 \pm 13.91 $\mu\text{g}/\text{m}^3$). The PM_{2.5} in Beijing was dominated by elements (35.9%), followed by carbonaceous species (OC and EC) (27.9%) and ions (21.7%). In the case of the PM_{2.5} at Gwangju, ionic components (49.6%) has the highest fractions, followed by carbonaceous species (20.4%) and elements (10.9%). Significant different chemical characteristics were found between two urban sites with the higher fractions of Ca²⁺, Mg²⁺, Cl⁻, and K⁺ in ions, Ca, Fe, Si, Mg, and Al in elements, PAHs, hopanes and steranes, alkanes, and cycloalkanes in organic compounds, and CHON and CHN organic groups with higher S/C, and N/C ratios at Beijing site, while the Gwangju site had the higher fractions of NH₄⁺ and NO₃⁻ in ions, S, Br, As, Zn, and Pb in elements, acids, sugar/levoglucosan, and cholesterol in organic compounds, and CHO organic group with higher H/C and O/C ratio. Those differences suggest that fine particles at Beijing were affected by various combustion sources such as biomass burning, coal burning and traffics, and dust, and that the type of organics was dominated by primary (fresh) one, while biomass burning and traffics mainly affected the Gwangju site with secondary (aged) organics dominant. Three types of haze events (NO₃⁻, Cl⁻, and K⁺-dominant event, EC, K⁺ and Cl⁻-dominant event, and dust-dominant event) were observed at Beijing site with increased acids, PAHs with higher benzene rings, sugar/levoglucosan, and CHN organic group were observed. At Gwangju site, one type of haze event (NO₃⁻, Pb, and K-dominant event) was observed with the increased sugar/levoglucosan, PAHs with higher benzene rings, CHON, CH, and CHNS organic groups compared to those during non-haze days. The increased emission strengths of various sources (biomass burning, coal burning, traffics, and dust) and secondary formation under stagnant conditions contributed to the winter haze events at the Beijing site. Also, the increased contributions of biomass burning and traffic sources and secondary formation under stagnant conditions contributed to the Gwangju haze events.

2UA.10**Characterization of Submicron Aerosols in a High Polluted City Nearby the Gorge of the Yellow River in Central China.**

QINGQING WANG, Yele Sun, Jie Li, Yong Chen, Yanyu Li, *Institute of Atmospheric Physics Chinese Academy of Sciences*

Although air pollution problem in megacities in China has been significantly improved as annual average PM_{2.5} in 2018 in Beijing was 51 $\mu\text{g}/\text{m}^3$. It is still a serious problem in many smaller cities. Sanmenxia is located in Fen-Wei Plain, close to China's largest coal base and nearby the gorge of the Yellow river. The highly concentrated industries, especially coal industries, heavy traffic, and the typical terrain of the gorge, make Sanmenxia a highly polluted city. Besides, elevated point sources from industrial chimneys circulated to the ground by local atmospheric circulation, which also aggravated air pollution. Nonrefractory PM₁ (NR-PM₁) species including organic aerosol (Org), sulfate (SO₄), nitrate (NO₃), ammonium (NH₄) and chloride (Cl) were measured at Sanmenxia Environmental Protection Bureau (34.794°N, 111.171°E) by the ACSM at a time resolution of ~5 min from December 21, 2018 to January 21, 2019. High time resolution of online meteorological variables, as well as precursor gases, OC/EC, and trace elements were also collected at the site, aiming to characterize the pollution sources and evolution mechanisms of aerosol chemical composition. A long haze episode lasted for 16 days was observed with NR-PM₁ = 76 \pm 33 $\mu\text{g}/\text{m}^3$, PM_{2.5} = 180 \pm 89 $\mu\text{g}/\text{m}^3$, indicating the severe polluted issue in Sanmenxia. During this episode, nitrate accounted for 32% of NR-PM₁ and was the primary species for NR-PM₁. Positive matrix factorization (PMF) analysis of both the ACSM organic mass spectra data and all other aerosol species showed the following sources in Sanmenxia: industrial emission, coal combustion, traffic emission, biomass burning, industrial point sources, secondary species (sulfate + nitrate + ammonium + secondary organic aerosol), and dust. The primary two sources were secondary species and coal combustion.

2UA.11

Micro-environmental Impact of a Proposed "Tri-gen" Facility in a Large Food Distribution Center. BO YANG, Murari Iyengar, Jeffrey Sward, K. Max Zhang, *Cornell University*

Megacities tend to put the wholesale markets together. A typical case is the Hunts Point Food Distribution Center (FDC) in Bronx, NY, which is \$2 to 2.3 billion industry supplying 25% of produce, 35% of meat, and 45% of fish consumed in New York City. FDC has diverse energy needs, including heating for the meat market and the local heating network, cooling for the produce market, and electricity. However, the current energy supply is separated and inefficient. A combined cooling, heat, and power (CCHP) facility, also known as "tri-gen", has been proposed at the FDC, which could efficiently generate three types of energy together. In this study, we assessed the local air quality impact at Hunts Point before and after introducing the CCHP facility. The "before" scenario included two gas-fired steam boilers (20 MMBtu/hr each) and 360 diesel-powered transport refrigeration units (TRCs). In the "after" scenario, the two gas-fired steam boilers and 50% of the TRCs were replaced by a 5.2 MW CCHP facility. The ground-level concentrations (GLCs) were predicted and analyzed by using Computational Fluid Dynamics (CFD) simulations. We reported significant improvement in micro-environmental air quality due to the CCHP facility, which could result in substantial occupational health benefits.

2UA.12

Mobile Measurements to Identify Spatial and Temporal Variability of Aerosol Composition during the NAMaSTE Campaign. Benjamin Werden, Erin Katz, Michael Giordano, Siva Praveen Puppala, Elizabeth Stone, Robert J. Yokelson, Donald Blake, Arnico Panday, PETER DECARLO, *Drexel University*

During the Nepal Ambient Monitoring and Source Testing Experiment (NAMaSTE), mobile measurements of aerosol composition were made using a "mini" Aerosol Mass Spectrometer. Fourteen separate drives were conducted in the Kathmandu Valley with the goal of assessing differences in aerosol particle composition over the spatial extent of the valley and at different times of the day. East-west transects of the valley started south of Kathmandu, and proceeded to the ring road, and then east through the peri-urban areas followed by the high brick kiln region of Bhaktapur, and finally to the valley edge in Dhulikhel. North/south transects similarly started at ICIMOD south of Kathmandu, and proceeded North following the ring road and then terminating at the base of the mountains north of the city. These drives captured large differences in concentration and composition of ambient aerosols that can be attributed to strong source emissions that are spatially distinct combined with meteorology directing plumes to some areas of the valley, but not others. Organics were by far the largest contribution to total aerosol particle mass, and showed chemical signatures from primary emissions including traffic, biomass burning and trash burning. Inorganic species such as sulfate and chloride were useful in separating influence from brick kilns, and trash and agricultural burning.

2UA.13

Characterization of Particulate Bound Polycyclic Aromatic Compounds (PACs) and Their Oxidations in Heavy Polluted Atmosphere: A Case Study in Urban Beijing, China during Haze Events. LIJUAN LI, Steven Sai Hang Ho, Junji Cao, *Chinese Academy of Sciences*

Characterizations on polycyclic aromatic compounds (PACs) during frequent haze periods have been conducted in an urban site of Beijing, China. Particulate polycyclic aromatic hydrocarbons (PAHs) and oxygenated-PAHs (OPAHs) and other carbonaceous matters were quantified. The average $PM_{2.5}$ during haze events ($256.3 \pm 103.7 \mu\text{g}/\text{m}^3$) were one magnitude over than that of CRs ($24.7 \pm 27.7 \mu\text{g}/\text{m}^3$). The average total quantified PAHs (ΣPAHs) and OPAHs (ΣOPAHs) during haze events were $423.9 \pm 178.4 \text{ng}/\text{m}^3$ and $581.4 \pm 299.8 \text{ng}/\text{m}^3$, respectively, which were 10 times higher than those of $40.3 \pm 68.2 \text{ng}/\text{m}^3$ and $54.4 \pm 82.4 \text{ng}/\text{m}^3$ in clear days. Four-rings PAHs had the highest compositions. 1,8-Naphthalic anhydride (1,8-NA) is the most abundant OPAHs, accounted for 49.8% of ΣOPAHs , followed by 9,10-anthraquinone (9,10-AQ) (13.8%) and benzo(a)anthracene-7,12-dione (BaAQ) (8.31%). In haze events, the contents of 5- to 7-rings PAHs decreased by 2.32% compared with those of clear days, while lower molecular weight fractions of 3- and 4-rings PAHs increased. The relationships between PAHs, OPAHs and relative humidity (RH) were found to be exponential. High oxygenation rate (R_0) ratios of OPAH /PAH represents higher rates in secondary formation or degradation and gas- particle conversion for each PAH or OPAH during the wintertime. Significant positive correlation between BeP and OPAHs ($r=0.97$), combined with the results of photochemical aging and negatively correlation with O_3 , suggest that secondary atmospheric reactions of PAHs played an important role in the burden of OPAHs.

2UA.14

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 the 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 February 2017 and July 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 and solving the general dynamic equation for aerosol microphysics. Model inputs include traffic emissions at 1 km resolution, spatially resolved using a traffic model for Pittsburgh. Baseline simulations indicate February 2017 particle number concentrations (PNC) in Pittsburgh vary by more than a factor of two, with a mean concentration of $9,000 \text{cm}^{-3}$. Comparisons to a network of 27 long-term (~1 month) winter observation sites in Pittsburgh show model spatial agreement with MFB = -15% and MFE = 22% at 13 urban background and local sites. At 14 sites influenced by local sources or topography, there is poorer agreement with MFB = -39% and MFE = 39%, indicating the importance of local sources and variability that are not resolved even at 1 km model resolution. Temporally, the model matches winter diurnal variability in PNC at 12 sites with r^2 values exceeding 0.29. Sensitivity simulations to quantify source apportionment show on-road traffic contributes to 29% of predicted PNC within Pittsburgh followed by both stationary wood combustion and waste disposal at 17%. We estimate natural gas combustion to contribute 15% of predicted PNC. Using a traffic model to spatially allocate traffic emissions inputs captures the traffic patterns better: predicted NO_2 at 46 distributed NO_2 observation sites across Pittsburgh yields higher agreement ($r^2 = 0.39$, MFB = -13%, MFE = 21%) than simulations at default EPA spatial surrogates ($r^2 = 0.29$, MFB = -27%, MFE = 51%). Primary emissions largely govern the spatial variability in predicted PNC at the 1-km scale. Mean predicted particle lifetime due to coagulation is 10 hours within the city with only 7% of particles lost due to coagulation. Modeling at 1-km resolution resolves more variability in human exposure. The 5th-95th percentiles of population were estimated to be exposed to $3,400\text{--}8,700 \text{cm}^{-3}$ at 1 km resolution, but $3,500\text{--}7,000 \text{cm}^{-3}$ at 4 km resolution.

2UA.15**Elevated Number and Mass Concentrations of Fine Particles during Winter in 2018 and 2019 in Urban Gwangju, Korea.**

JIHO JANG, Haebum Lee, Nohhyeon Kwak, Minhan Park, Jiho Chong, Ma. Cristine Faye Denna, Kihong Park, *Gwangju Institute of Science and Technology*

Fine (<2.5 μm) and ultrafine (<100 nm) particles are of current interest due to their effects on radiation balance, cloud formation, and human health (Takami et al., 2005). It is important to understand source and formation pathways for fine and ultrafine particles elevated in urban ambient atmosphere (Song et al., 2010; Wagstrom and Pandis, 2011). An intensive measurement was conducted during the winter of 2018 (1/3-2/2) and 2019 (12/27-01/25) at urban Gwangju, Korea (35.23° N, 126.84° E). Particle number concentrations of fine and ultrafine particles were measured with a scanning mobility particle sizer (SMPS) which includes differential mobility analyzer (DMA) (3085, TSI, USA) and condensation particle counter (CPC) (3022, TSI, USA), and an optical particle counter (OPC) (1.108, Grimm, USA). The mass concentration of black carbon (BC) and particulate matter (<2.5 μm) were measured with an aethalometer (AE-31, Magee, USA), and OPC, respectively. Average number concentrations (particles/cm³) of particles in size ranges of 20-100 nm, 20-700 nm, and 0.3-2.5 μm were 2355 (± 1452), 4038 (± 2085), and 159 (± 131), respectively. Average mass concentrations ($\mu\text{g}/\text{m}^3$) of PM_{2.5} and BC were 10.96 (± 3.85) and 1.19 (± 0.83), respectively. Twelve new particle formation (NPF) events (elevated number concentration of ultrafine particles (<100 nm) with subsequent growth) and seven PM_{2.5} event days (elevated PM_{2.5} mass concentration) were observed. It was found that NPF event days were not identical with the PM_{2.5} event days. Various characteristics of NPF and PM_{2.5} concentration events at urban Gwangju are being investigated.

2UA.17**Spatial Variation of Air Pollutants Using Machine Learning**

Models. JIAJUN GU, Gaurav Bang, Abhijeet Guha Roy, Michael Brauer, Benjamin Barratt, Martha Lee, K. Max Zhang, *Cornell University*

Urban air pollution is characterized by significant spatial heterogeneity as a result of multiple emission sources, complex urban morphology and dynamic meteorology. In this study, we compared four different machine learning models, i.e., land-use (linear) regression (LUR), random forest (RF), Gaussian process (GP), and artificial neural networks (ANN) to predict the spatial variations of nitrogen dioxide (NO₂), nitrogen oxide (NO), PM_{2.5}, and black carbon (BC) concentrations in Hong Kong. LUR uses a linear predictor function and is easy to interpret, but is difficult to capture the non-linear relationships and can lead to variance inflation due to multicollinearity. RF constructs a number of decision trees and outputs the mean predictions of the individual trees, which can capture non-linear relationships, but has the drawback of model interpretability. GP takes a stochastic view with the key idea of imposing a multivariate Gaussian prior distribution over the functions reflecting the input-output relations. It takes advantage of the nonparametric flexibility and is able to quantify the uncertainty, with the cost of computation time. ANN models the interdependence among all the predictors and is able to capture complex relationships. Its main drawback is model interpretability due to its black-box nature. All the models were evaluated using hold-out evaluation, with different percentages of sites held out. In terms of prediction accuracy, ANN outperformed RF and GP, and LUR ranked the last. But ANN's black-box nature also made it the least interpretable. We argue that GP is advantageous when prediction accuracy and model interpretation are equally important. Also, GP's nonparametric flexibility and capability to quantify uncertainties hold great promise in a variety of air pollution applications.

2UA.19

Ambient Air Quality in Urban Areas of Indonesia. Muhayatun Santoso, Diah Lestiani, Syukria Kurniawati, ENDAH DAMASTUTI, Djoko Prakoso, Indah Kusmartini, Rita Mukhtar, Philip K. Hopke, *Center for Applied Nuclear Science and Technology, BATAN*

This research was conducted to assess the air quality in 16 urban areas of Indonesia covering Java, Sumatera, Kalimantan, Sulawesi, Maluku, and Papua islands. Samples of fine ($PM_{2.5}$) and coarse fractions ($PM_{2.5-10}$) of airborne particulate matter have been collected using a Gent stacked filter unit, once a week for 24hrs, from January 2014 until the present. More than 1500 pairs samples were collected. The samples were analyzed for mass, black carbon, and elemental composition. Nuclear techniques have been used in quantification of environmental pollutant. The results showed that majority of the annual concentrations of $PM_{2.5}$ in 6 sites of Java islands exceeded the Indonesian annual air quality standards ($15 \mu\text{g}/\text{m}^3$), while that of PM_{10} were lower than its daily guideline value ($150 \mu\text{g}/\text{m}^3$). The overall air quality in the urban sites of Java islands (Jakarta, Tangerang, Bandung, Yogyakarta, Semarang, Surabaya) were higher compare to other sites in other islands of Indonesia. The average ratio of BC concentrations compared to the $PM_{2.5}$ concentrations ranged from 12 to 24 %. Several compositions of elemental concentrations were also determined. The results obtained in Surabaya and Tangerang sites showed that level of lead and some other heavy metals in $PM_{2.5}$ significantly higher than in other sites. The maximum of lead concentration at Surabaya and Tangerang sites reaches tens of times higher than US EPA NAAQS ($0.15 \mu\text{g}/\text{m}^3$), while the average of Zn concentrations in Surabaya were more than 3 times higher than other sites in Java, and tens of times higher than other sites outside Java. Air quality during volcanic eruption and forest fires in these sampling periods will also be discussed comprehensively. The results obtained from this research gave very important information as early warning and scientific research-based references to avoid greater financial disadvantage and human health impact. Better solution and proper action should be taken into this matter.

2UA.20

Chemical Composition, Sources and Formation Process of Submicron Aerosols in Seoul Metropolitan Area during Summer: Comparison to Winter. HWAJIN KIM, Qi Zhang, *Korea Institute of Science and Technology*

To investigate the seasonal characteristics of submicron aerosol (PM_1) in urban Korea, characteristics of PM_1 were investigated using an HR-ToF-AMS in the Seoul Metropolitan Area (SMA) during summer. Also by applying positive matrix factorization (PMF), organic aerosol (OA) sources were investigated and the results were compared to the one in winter.

In summer, the average concentration of PM_1 was $19.1 \mu\text{g m}^{-3}$, which was composed of 49% organics, 28% SO_4 , 7% NO_3 , and 9% NH_4 . And eight distinct sources of OA were identified: hydrocarbon like OA (HOA), cooking OA (COA), nitrate OA (NO_3 -OA), sulfate OA (SO_4 -OA), nitrogen enriched OA (NOA) and three different levels of oxidized OA (OOA1, OOA2, OOA3).

Compared to winter, the average PM_1 concentration was lower during summer (19.1 vs $27.5 \mu\text{g m}^{-3}$), the mass fraction of SO_4 was higher (28 vs. 10 %) but that of NO_3 was lower (7 vs 24 %). Together with lower SO_2 in summer (4.3 vs 6.9 ppb), higher SO_4 concentration (5.4 vs $2.9 \mu\text{g m}^{-3}$) indicate the more efficient conversion of SO_2 to SO_4 under stronger solar radiation (0.95 vs $0.66 \text{ MJ}/\text{m}^2$) or more regional transport of sulfate. Furthermore, PMF analysis indicate that about 20% of SO_4 during summer is in organic combined. In terms of OA, OA was more oxidized (O/C ratios; 0.46 vs 0.37) and more different types of SOA sources (6 vs 2) were observed, composing higher SOA fraction than the one in winter (80 vs 41%). One reason for this is the intensive photochemical formation occurred in summer showing the better ($r=0.65$ vs 0.47) and higher daytime OOA/ O_x ratios (0.17 vs 0.12). Also the impact of POA was less in summer. These results indicate that air quality in SMA reflect the differences between the two seasons in meteorology, emissions sources and formation processes of air pollutants.

2UA.21

Comprehensive Mobile Measurements of Aerosols from Residential Heating in Small Settlements for Temporal/Spatial Variability and Hot-Spots Identification: Cross-Border Study. JAN BENDL, Jan Hovorka, Jürgen Schnelle-Kreis, Gert Jakobi, Mohamed Khedr, Xiansheng Liu, *Charles University*

Residential heating represents in Middle/Eastern Europe serious health risk especially in small settlements during winter-time. The air pollution models mostly lack data from microscale, so PM is underestimated. Moreover, boilers and stoves are hardly regulated by states and citizens are not aware.

We developed an appropriate methodology for comprehensive mobile aerosol temporal/spatial variability observation in small settlements where the same 1-hour long route across the village with strollers (inlets in the breathing zone) is repeated 8 times a day (5am–10pm).

PM_{1, 2.5, 10}, Particle size distribution, PNC (1 second integration time), BC (10 sec) concentration are plotted into maps. The aerosol is sampled during the whole route in 2 fractions for PAHs analysis (IDTD-GC-TOF-MS). Low-cost PM devices are tested for future citizen-science applications.

We conducted simultaneous measurements (11/22-25/2018) by two strollers in two similar-sized villages, 2.5 km far from each other in the Czech-German border area – Zelezná Ruda (Czechia) and Bayerisch Eisenstein (Germany). Surrounding national park ensured isolation from other sources and three stationary PM_{2.5} instruments with meteo-station recorded dynamics of background.

Overall higher concentrations during the same atmospheric conditions were measured on the Czech side due to more coal and wood combustion boilers. The highest median of PM_{2.5} was during the walk on 24th November (6-7 pm) 444 µg.m⁻³ with peaks up to 11 mg.m⁻³ while in Germany was median 61 µg.m⁻³. High temporal and spatial variability was observed, PM_{2.5} ranged in two orders of magnitude during one walk (plumes) which suggests mobile measurements are an appropriate method for real personal exposure and hot-spots identification in small settlements.

The study is supported by the DSPF PA06 Project “CONSPIRO – Breathing Together” coordinated by EC-JRC (TFAQ).

2UA.22

Efficacy of an Engineered Vegetative Buffer on Near-Road Air Quality. PRADEEP S. PRATHIBHA, Ray Yeager, Aruni Bhatnagar, Daniel Fleischer, Brent Bucknum, Eben Cross, Jay R. Turner, *Washington University in St. Louis*

Exposure to urban air pollution is a major risk factor for cardiovascular and respiratory diseases, and urban greening is a proposed means of reducing near-road air pollutant levels and improving public health. In this study, real-time gaseous pollutant and particulate matter concentrations were monitored on multiple days at an engineered vegetative buffer planted adjacent to a principal arterial road (annual average daily traffic: 33,515). The buffer, nominally 12 m deep and 75 m long, was designed by Hyphae Design Laboratory (Oakland, CA) with shrubs and forbs nearest to the road, followed by woody trees, to maximize pollutant dispersion and deposition.

Field monitoring featured three mixing condensation particle counters (MCPCs, Brechtel Inc., Hayward, CA) simultaneously measuring 1-second ultrafine particle (UFP) concentrations at the Road (10 m from edge of the road), Control (35 m from the edge of the road in an open fetch), and Buffer (35 m from edge of the road, 15 m behind the buffer). During crosswinds approaching the buffer from the road, the median reduction in 3-min averaged UFP concentration at the Buffer was 15% (1,100 particles/cc) lower than at the Control. The buffer reduced wind speed by up to 50% (1.2 m/s), with the reduction plateauing with increasing wind speed. 5-sec estimated particulate matter mass concentrations data, measured using OPC-N2 optical particle counters (Alphasense Ltd, Essex, United Kingdom) aboard ARISense nodes (Aerodyne Research, Inc., Billerica, MA), are also being analyzed for buffer effects.

This pilot study is informing the design of a community-scale prospective study, Green Heart Louisville (louisville.edu/greenheart), to examine linkages between urban vegetation and cardiovascular health, an association potentially mediated by the effect of vegetation on local air quality.

2UA.24

A Topic Model Approach and Its Implication on Particulate Matter Related Research: A Case for South Korea. KAYOUNG KIM, *KISTEP*

One of the biggest and constant issue in South Korea is Particulate Matter (PM) pollution for several years now. The concern of the public is rapidly increasing because of that PM is designated as carcinogenic substances by WHO and in numerical and visually as well that the situation is hardly getting better, particularly in PM_{2.5} concentrations. In 2017, the government announced the 'PM Response Strategy Based on Science and Technology (FY2017 -2023)' and continue to expand its R&D budget. The R&D budget for PM area is about KRW 94.2 billion in FY2018 which is about 37.0% increase over the last three years. As its R&D projects are conducted competitively that there is a concern about likely to have an overlapping investment and inefficiency. The purpose of this study is to examine how PM pollution area has evolved in South Korea and globally. Based on the technology category from the policy, we have gathered 536 South Korean R&D projects and 9,260 SCI paper data from 2015 to 2017. The research conducted topic model analysis to chronological and by country, particularly South Korea and China, the changes of main key words in this research field. As a result, it is expected to use as basic data for budget allocation process, policy implication, and international cooperation on PM response strategy.

2UA.25

Can Nucleation in the Residual Layer Explain “Class-B” New Particle Formation Events? NICHOLAS MESKHIDZE, Juan Jaimes-Correa, Markus Petters, Taylor Royalty, Brittany Phillips, Alyssa Zimmerman, Robert Reed, *NC State*

The sources and sinks affecting ambient concentrations of ultrafine particles ($D_p < 100$ nm) are a topic of interest in air quality and climate sciences. New particle formation is a secondary source of ultrafine particles. Different types of new particle formation events have been observed. During Class-A events, nucleation mode particles are starting with molecular clusters ~ 1.5 nm in size, followed by continuous modal growth. During Class-B events, particles also grow, but the first detected particle mode exceeds 10 nm. The lack of observed sub-10 nm sized particles during Class-B events has been interpreted as that nucleation happened upwind of the measurement site. Here we propose a different explanation for the observed size distributions during Class-B events. Size distributions were measured in Raleigh, NC, during November–December 2017. Five well-defined Class-B events that lead to a broad regional scale increases in ultrafine particle concentration were observed. Data analysis involving the time series of particle number size distribution, meteorological variables, air parcel back trajectories, surface weather maps, gas-phase chemical composition (i.e., CO, SO₂, NO, NO₂, O₃), and particle tracers (i.e., refractory black carbon, non-hygroscopic particles, condensation sink, PM_{2.5}, and PM₁₀) suggests that the nucleation events may have occurred inside the residual layer. The sudden appearance of nucleation mode particles could then be explained by turbulent mixing related to the growth of the daytime boundary layer, which results in downward mixing of particles that nucleated aloft and grew prior to vertical transport. This process leads to an increase in ultrafine particles during late morning/mid-day, a time when contributions from traffic to ultrafine particles are less.

2UA.26**Exploring the Spatiotemporal Variability of the Ground Level Ultrafine Particle Number Concentration in the Raleigh Area.**

Nicholas Meskhidze, Juan Jaimes-Correa, Markus Petters, Taylor Royalty, Brittany Phillips, ALYSSA ZIMMERMAN, Robert Reed, *North Carolina State University*

Ultrafine particles (UFP), aerosols with diameters less than 100 nm, are known for their impact on human health and the Earth's energy balance. Relatively few studies have investigated sources and sinks, as well as, diurnal, weekly, and spatial variation of UFP number concentration in the urban and suburban environment of Raleigh, NC. The measurement campaigns have been carried out at the urban (Nov-Dec 2017) and suburban (Nov-Dec 2018) sites in Raleigh to characterize number size distribution and hygroscopicity of UFPs. The urban site was located at NC State University campus, at the intersection of two roads with heavy traffic, including light passenger cars, heavy-duty trucks, and university-owned diesel buses. The suburban site was located 15 km south from the urban site, at the Lake Wheeler Road Facility. The site is located over the flat grassy terrain and is surrounded by NCSU's animal science, crop and soil science, biological and agricultural engineering research facilities, and animal and poultry waste management processing facility.

Our data analysis involving the time series of particle number size distribution, meteorological variables (i.e., pressure, temperature, RH, wind speed and direction, solar radiation, and precipitation, the gas-phase chemical (i.e., CO, SO₂, NO, NO₂, O₃), and particle tracers (i.e., refractory black carbon, non-hygroscopic particles, condensation sink, PM_{2.5}, and PM₁₀) revealed two distinct sources of UFPs associated with vehicle emissions and broad background nucleation. The current presentation will discuss the spatiotemporal variability of UFP number size distribution and highlight the important role of local meteorology (and in particular the boundary layer dynamics) for determining the ambient air pollution levels in the Raleigh area.

2UA.27**Comparison of Organic Compounds in PM_{2.5} High-Concentration Events from Seoul and Beijing.**

HYEWON KIM, Soyoun Jung, Jieun Park, Youngkwon Kim, Seung-Muk Yi, Kwang-Jo Moon, Kwon Ho Jeon, *Seoul National University, Seoul, Korea*

Seoul and Beijing are both megacities with high population and traffic volume. These two cities are highly polluted due to the local air pollution from primary sources such as industrial complexes as well as the inflow of air pollutants from other East Asian countries. In particular, fine particulate matter (PM_{2.5}) from high-concentration events (HCEs) that occur in winter and spring contains various organic compounds.

Organic carbon, which comprises 20-80% of the total mass of PM_{2.5}, consists of various organic compounds, which exhibit characteristics that are related to emission from specific sources such as mobile and coal combustion. To develop control strategies against PM_{2.5}, contributing sources can be determined by identifying the chemical properties of these organic compounds. Although the main compositions of PM_{2.5} for each city were reported in several studies, only a few studies compared organic compounds from both cities. Thus, the purpose of this study is to compare the characteristics of organic compounds in HCEs from both cities.

To determine the characteristics of organic compounds, PM_{2.5} samples were collected for 23-hr in Seoul and Beijing by using a high-volume air sampler (TE-HVPLUS, TISCH, USA). The collected samples were extracted with an organic solvent that contained a 3:1 mixture of dichloromethane (DCM) (HPLC grade, J. T. Baker, USA) and methanol (HPLC grade, J. T. Baker, USA), and the extracts were concentrated with nitrogen gas to 1 mL by using TurboVap II (Caliper Life Sciences, USA). The final concentrates were analyzed for organic compounds such as polycyclic aromatic hydrocarbons (PAHs), n-alkanes and hopanes by gas chromatography/mass spectrometry (7890A/5975C, Agilent).

2UA.28

Air Quality and Health Co-benefits of Different Deep Decarbonization Pathways in California. BIN ZHAO, Tianyang Wang, Zhe Jiang, Yu Gu, Kuo-Nan Liou, Yifang Zhu, *University of California Los Angeles*

As the world's fifth-largest economy, California has committed to reduce its greenhouse gas (GHG) emissions by 80% below 1990 levels by 2050. The 2015 Paris Agreement further necessitates the target of net-zero GHG emissions. While previous studies have shown that GHG reductions could synergistically decrease air pollutant emissions, limited research has been conducted to compare the air quality and health co-benefits of different technology pathways towards deep decarbonization. Using an integrated approach that combines energy and emission technology modeling, high-resolution chemical transport simulation, and health impact assessment, we find that achievement of the 80% GHG reduction target would bring substantial air quality and health co-benefits. The co-benefits, however, highly depend on selected technology pathway largely because of California's relatively clean energy structure. Compared with the business-as-usual levels, a decarbonization pathway that focuses on electrification and clean renewable energy is estimated to reduce concentrations of fine particulate matter (PM_{2.5}) by 18-37% in major metropolitan areas of California and subsequently avoid about 12,100 (9,600-14,600) premature deaths. In contrast, only a quarter of such health co-benefits, i.e., 2,800 (2,300-3,400) avoided deaths, can be achieved through a pathway focusing more on combustible renewable fuels. After subtracting the cost, the net monetized benefit of the electrification-focused pathway still exceeds that of the renewable fuel-focused pathway, indicating that a cleaner but more expensive decarbonization pathway may be more preferable in California. Achieving net-zero GHG emissions beyond the 80% reduction target requires bioenergy with carbon capture and sequestration (BECCS) technology to offset some GHG emissions. BECCS technology, whereas supporting the net-zero target, would emit considerable air pollutants and increase about 400 premature deaths, suggesting a potential trade-off between climate benefits and health co-benefits of ambitious climate policies.

2UA.29

Validating the Intervention Model for Air Pollution for Environmental Health and Justice Analysis in Canada. RIVKAH GARDNER-FROLICK, Christopher Tessum, Julian Marshall, Amanda Giang, *University of British Columbia*

Reduced complexity air quality models are valuable for predicting pollutant concentrations while requiring less computing power and being more accessible to diverse knowledge users than traditional chemical transport models. The Intervention Model for Air Pollution (InMAP) is one such model that uses simplified chemistry and physics, paired with health impact formulas, to focus on the health impacts of fine particulate matter (PM_{2.5}) and the distribution of impacts across populations. The model uses a variable grid with up to 1-km resolution, enabling estimates of urban exposures while still covering a large spatial domain. These characteristics make InMAP especially useful for a variety of applications, including those that aim to investigate environmental justice questions, those that necessitate many model runs, and projects that cannot use chemical transport models.

Currently, the InMAP domain includes Canada as part of the emissions scenario for the United States. However, the model has not yet been validated in Canada and has not been run with Canada-specific data. This project validates InMAP estimates against measured concentrations of PM_{2.5} and other criteria pollutants at Canadian government monitoring stations. In addition, the project validates InMAP results when the model is instead run with Canadian emissions and demographic data. Updating the model to include Canada-specific emissions and demographic data will enable InMAP's use to answer uniquely Canadian environmental justice questions about PM_{2.5} exposure and distribution among vulnerable populations.

2UA.30**Spatiotemporal Profiles of Ultrafine Particles Differ from Other Traffic-Related Air Pollutants: Lessons from Long-Term Measurements at Fixed Sites and Mobile Monitoring.**

SHAHZAD GANI, Sarah Chambliss, Kyle Messier, Melissa M. Lunden, Joshua Apte, *University of Texas at Austin*

The health risks of ultrafine particle (UFP, $D_p < 100$ nm) exposure are an important subject of current investigation in air pollution epidemiology. With routine monitoring of UFP still uncommon, health studies often use other pollutants as proxy for UFP. Here, we use two rich datasets — one with high spatial coverage, and the other with high temporal coverage — to investigate how the spatial-temporal patterns of UFP relate to other traffic-related air pollutants, especially NO_x . We incorporate 3–6 years of hourly particle number (PN) concentration data from multiple fixed sites across the San Francisco Bay Area that include near-highway, urban, suburban and rural sites. In addition, we incorporate observations from a 32-month mobile monitoring campaign comprising >3,000 h of coverage of a range of road types and land uses.

Overall annual-average PN at the fixed sites span a range of $3 \times 10^3 \text{ cm}^{-3}$ at rural site to $30 \times 10^3 \text{ cm}^{-3}$ at near-highway site. Across all sites, PN measurements on nearly all summer days show consistent, prominent mid-day peaks, lasting 5–7 h. This diurnal concentration pattern—characteristic of new particle formation — is not observed for other co-emitted pollutants (NO_x , BC, CO). While we found moderate correlation in diurnal patterns of NO_x and UFP at sites with high traffic, the correlation dropped significantly for low traffic areas — especially during high insolation (e.g., summer daytime) periods. Mobile monitoring data yielded similar results: NO_x was observed to have weaker correlations with UFP for non-highway roads during high insolation periods. UFP in urban atmosphere is known to result primarily from vehicular traffic and photonucleation events. As a result, the spatiotemporal profiles of UFP can differ strongly from other traffic-related air pollutants when new particle formation from photonucleation contribute to a significant fraction of UFP.

2UA.31**Ten-year Trends (2008–2017) in Ambient Fine Particulate Matter and Its Chemical Components in the Capital Region of New York State.** SANCHITA PAUL, Md. Aynul Bari, *University at Albany, SUNY*

With ongoing interest and concern about the state of fine particulate air pollution in U.S. urban centers, a study was undertaken to investigate temporal trends in fine particulate matter ($\text{PM}_{2.5}$) and its chemical components in Albany, NY over a 10-year period (2008–2017). A non-parametric trend detection method based on Mann-Kendall with Thiel-Sen's slope was applied to estimate trends using annual geometric mean concentrations. A weak downward trend (significant at 90% confidence level) was found for ambient $\text{PM}_{2.5}$ concentrations with an annual decrease of $-0.23 \mu\text{g}/\text{m}^3$ (–3%) per year. Statistically significant decreasing trends were observed for secondary species such as particulate sulfate ($-0.14 \mu\text{g}/\text{m}^3$, –8% per year), nitrate ($-0.04 \mu\text{g}/\text{m}^3$, –6% per year) and ammonium ($-0.07 \mu\text{g}/\text{m}^3$, –10% per year). Among carbonaceous aerosols, significant downward changes ($-0.02 \mu\text{g}/\text{m}^3$, –4% per year) were observed for elemental carbon (EC), while no significant changes were detected for organic carbon (OC). These observed changes are primarily due to several emission reduction strategies for light- and heavy-duty vehicles and power generation that have been adopted across NYS since 2000 including particle regeneration traps and NO_x control on heavy-duty diesel on-road trucks, reduction of sulfur in off-road diesel fuels, and use of ultralow sulfur in distillate fuels. A statistically significant increasing trend was observed for copper ($0.23 \text{ ng}/\text{m}^3$, 14% per year) suggesting the influence of non-exhaust road traffic emissions. Concentrations of K^+ , Zn , Cl^- showed significant seasonal variability with higher concentrations in winter than in summer likely reflecting wood smoke origins more than other potential sources in Albany surrounding region. No statistically significant changes were found for all other chemical components examined. Longer-term $\text{PM}_{2.5}$ speciation data at least over several decades are needed to establish whether trends reported here actually occurring.

2UA.32

Onshore Measurements of Emissions from In-Use Tugboats in Southern California. HANNAH SCHLAERTH, Joseph Ko, Rebecca Sugrue, Chelsea V. Preble, Thomas W. Kirchstetter, George Ban-Weiss, *University of Southern California*

Black carbon (BC) emitted from diesel fuel combustion contributes significantly to total particulate matter (PM) emissions that impact air quality and human health. As on-road sources of PM decline due to the wide adoption of emissions control technologies on diesel trucks, understanding off-road emissions sources is becoming more important to further reduce total PM emissions. Tugboats spend most of their operational time near the coast maneuvering large vessels in and out of berth, making them important contributors to near-shore air pollution. However, few studies have measured emission rates from this source-type, and none have successfully investigated how operational parameters affect their emissions. Measurements of emission rates from tugboats are needed to improve and update official governmental emissions inventories for marine vessels, especially since the few measurements that have been made suggest high vessel-to-vessel emissions variability.

Emissions from in-use tugboats were measured from shore as vessels passed by a pier in the Port of Long Beach in Southern California using the plume capture method. BC concentrations were measured using a single particle soot photometer and a custom-built aerosol black carbon detector. Particle number, PM_{2.5}, and CO₂ concentrations were measured, respectively, using a model 3007 TSI Condensation Particle Counter, a handheld DustTrak DRX, and a Li-Cor 840a. Fuel-based emission factors were calculated by carbon balance for the three operating modes observed: cruising against current, cruising with current, and towing vessels. Observed emissions variability within the fleet was analyzed by vessel dimensions, build years, and engine power when Automatic Identification System data was available. Preliminary results suggest that BC emission factors from measured tug boats ranged from near-zero to ~1 g/kg, with a mean (\pm standard deviation) BC emission factor of 0.52 ± 0.37 g/kg. This study offers unique insight into the emission rates of the Southern California tugboat fleet because of the large sample size of unique vessels and repeated observations for vessels under multiple operating conditions.

3AC.1

Application of a Reactive Uptake Parameterization Considering Non-Ideal Effects and Phase State in Simulating Secondary Organic Aerosols from Isoprene Epoxydiols Under Controlled Laboratory Measurements. YUZHONG CHEN, Yue Zhang, Matthieu Riva, Theran P. Riedel, Havala Pye, Nicole Olson, Ziyang Lei, Zhenfa Zhang, Avram Gold, 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) in the presence of acidic sulfate-containing aerosols within the atmosphere. IEPOX-derived SOA can contribute up to 40% of OA mass in isoprene-rich regions such as the southeastern U.S. Representing efficiency of uptake by a coefficient (γ_{IEPOX}) has been convenient for predicting IEPOX-SOA in chemical transport models. However, large uncertainties are associated with such approach. A laboratory study has shown that the available condensed-phase reaction-rate constants are likely under-predicted as they fail to predict the extensive conversion of inorganic sulfate to organic sulfate by IEPOX. The substantial formation of surface-active organosulfates results in a particulate morphology with a viscous organic-rich shell surrounding an aqueous inorganic core. Consequently, acid-driven reactive uptake of IEPOX is inhibited by the growing organic shell over time. This so-called “self-limiting” effect, along with the potential under-prediction of kinetic parameters has yet to be investigated in a controlled environment.

In this work, time-resolved condensed-phase concentrations of IEPOX-SOA molecular tracers were obtained from chamber experiments conducted with authentic *trans*- β -IEPOX and acidic sulfate aerosols. A one-dimensional box model considering the “self-limiting” effect was used to derive and evaluate reactive uptake parameterization against measurements. Newly derived condensed-phase reaction-rate constants forming major SOA tracers were found to be at least 2 orders of magnitude higher than those used in the current models, consistent with those derived from computational chemistry. Sensitivity analyses were performed, and recommended values were given for other relevant parameters, including Henry’s law constants and IEPOX diffusion coefficient in the organic shell of IEPOX-SOA. Current air quality and global models need to be updated to assess the improved parameterization derived from this work, which is critical to understanding the processes that govern formation of IEPOX-SOA in the atmosphere and developing air-pollution mitigation strategies.

3AC.2

Modeling the Effects of an Updated Isoprene Oxidation Mechanism on Organic Aerosol, Reactive Nitrogen, and Sulfate Budgets. KELVIN BATES, Eleni Dovrou, Vasquez Krystal, Frank Keutsch, Paul Wennberg, Daniel Jacob, *Harvard University*

We implement the Reduced Caltech Isoprene Mechanism (RCIM), a recently developed state-of-the-science gas-phase isoprene oxidation mechanism, into the global chemical transport model GEOS-Chem and investigate its global effects of secondary organic aerosol (SOA) formation. We find an SOA yield from isoprene of 13% per carbon, much higher than commonly assumed in models, and likely offset by SOA chemical loss through aging mechanisms not yet included in GEOS-Chem. Global production of isoprene SOA is about one third each from isoprene epoxydiols (IEPOX), organonitrates, and C₅ tetrafunctional compounds, with much smaller contributions from glyoxal, methylglyoxal, and hydroxymethyl-methyl- α -lactone (HMML). Furthermore, through their interactions with inorganic components of aqueous particles, organic products of gas-phase isoprene oxidation can also play important roles in the budgets of particulate sulfur and nitrogen. Here, we present results from targeted experimental and field observations of two such interactions, along with simulations of their global impacts. First, using synthetic standards of isoprene-derived hydroperoxides (two isomers of C₅ hydroxyhydroperoxides, ISOPOOH, as well as hydroxymethyl hydroperoxide), we show that the oxidation of SO₂ to sulfate by organic hydroperoxides can proceed at atmospherically relevant rates in aerosol and cloud water due to the compounds’ high solubility and reactivity. Second, by comparing GEOS-Chem sensitivity simulations to ambient observations, we constrain the rapid hydrolysis of tertiary organonitrates ($\tau < 1$ s) in the aqueous phase, which converts reactive gas-phase nitrogen oxides into particulate inorganic nitrate. Finally, we perform GEOS-Chem global simulations with RCIM to show that both conversion of SO₂ to sulfate by organic hydroperoxides and removal of NO_x by isoprene hydroxynitrates play minor roles globally (<5% of total sulfate and nitrate formation), but can be significant (>50%) in areas with high biogenic VOC emissions, where these processes serve to decrease the availability of gas-phase H₂SO₄ for particle nucleation and NO_x for ozone formation.

3AC.3

Predicting the Phase State of Atmospherically Relevant Aerosols and Its Impact on Multiphase Chemistry in a Regional-scale Atmospheric Model. QUAZI RASOOL, Ryan Schmedding, Yue Zhang, Havala Pye, Haofei Zhang, Yuzhi Chen, Jason Surratt, William Vizuete, *University of North Carolina at Chapel Hill*

Accurate prediction of the phase state of secondary organic aerosols (SOA) is critical to quantify the impact on climate and air quality. Phase separation in SOA can create a highly viscous organic shell that surrounds an inorganic core, which can decrease both the partitioning of the semi-volatile species and the extent of acid-catalyzed heterogeneous reactions. Studies have showed that aerosols phase separate over 70% of the time at a rural site in the Southeast US by using observed compositions with thermodynamic models to predict organic and inorganic constituents as well as aerosol water content. However, such phase separation processes have not been fully incorporated into atmospheric models. This work developed algorithms for SOA phase separation that were included in a regional-scale atmospheric model (CMAQ). These new algorithms determine phase state by accounting for the mechanistic interactions between products of oxidizing precursor molecules, particle morphology, meteorology, and the aerosol water content. Our approach also estimates the glass transition temperatures (T_g) of SOA components by accounting the variability in composition of different organic compounds, aerosol water, and the atomic oxygen-to-carbon (O:C) ratio. When T_g determines a liquid state, we also included algorithms to determine whether there is Liquid-Liquid Phase Separation (LLPS), as recent literatures show that T_g provides a more accurate indication of phase separation that correlates well with the viscosity of SOA. Multiphase chemistry of isoprene-derived epoxydiols is one of the major sources of SOA in the troposphere. Our implementation is a first to focus on this critical pathway to estimate the impact of SOA phase separation on multiphase chemical reactions. To sum up, this work enables predictions of phase separation frequencies across varied conditions and subsequently examines the influence on isoprene-derived SOA phase separation due to aerosol viscosity, morphology, and phase state.

3AC.4

The Dependence of SOA Formation on NO_x Conditions: Effects of Branching Ratio of RO₂+NO Pathway. WEIHAN PENG, William Porter, David R. Cocker III, *University of California, Riverside*

Secondary organic aerosol formation is dependent on NO_x conditions because oxidation products of SOA precursors with different volatility form when NO_x condition varies. For example, during the photo-oxidation of aromatic compounds, low vapor pressure species form in peroxide rich (low-NO) conditions by favoring RO₂+HO₂ reactions and organic nitrates form in higher NO environments by favoring RO₂+NO reactions. Different NO_x indicators have been used to identify high and low NO_x conditions and quantify the effects of NO_x on SOA formation, including absolute NO_x concentrations, NO_x/VOC ratio, and HO₂/NO ratio. However, it is the branching ratio (β) of RO₂+NO reaction that determines composition and volatility of oxidation products from SOA precursors, because, instead of sole NO_x, NO_x/VOC or HO₂/NO, β decides the fraction of RO₂+NO reactions in RO₂ chemistry.

In this work, the global branching ratio distribution was estimated using the chemical transport model from GEOS-Chem. Four major categories of branching ratio ranges, as well as other environmental conditions including temperature and relative humidity, were simulated in the dual 90m³ environmental chamber at UCR/CE-CERT with the addition of typical anthropogenic or biogenic SOA precursors (xylene, α -pinene and isoprene). Volatility basis set mass yields for SOA products at different branching ratios were investigated and are in the process of being applied to a regional air quality model to improve the sensitivity and accuracy of SOA prediction at different NO_x conditions. Additionally, the bulk chemical composition of the aerosol formed was studied to improve the understanding of oxidation mechanism of SOA precursors at different branching ratios.

3AC.5

Translating Environmental Chamber Data for Secondary Organic Aerosol for Use in Atmospheric Models. CHARLES HE, Ali Akherati, Christopher Cappa, Jeffrey R. Pierce, ManishKumar Shrivastava, Benjamin Murphy, Shantanu Jathar, *Colorado State University*

For more than three decades, environmental chambers have been used as tools to study secondary organic aerosol (SOA) formation from volatile organic compounds (VOCs). Yet, SOA parameterizations based on chamber data may not appropriately account for the influence of multigenerational aging, losses of vapors to the chamber walls, varying NO_x levels, and phase state of the condensing SOA. In addition, parameterizations that are based on single compound studies may poorly represent the SOA formation from a mixture of lumped VOCs in atmospheric models. To address these problems, we used a state-of-the-science model to simulate the multigenerational chemistry, phase-dependent dynamic gas/particle partitioning, and vapor wall loss effects on SOA formation during chamber experiments. The chemistry and thermodynamic properties were modeled using the Statistical Oxidation Model (SOM) and the gas/particle partitioning kinetics were modeled using the Two Moment Aerosol Sectional (TOMAS) model. The SOM-TOMAS model will be used to develop SOA parameters for a host of anthropogenic (e.g., alkanes, aromatics) and biogenic (e.g., isoprene, monoterpenes) VOCs based on historical chamber data. Parameters will be determined by fitting the time series for SOA mass concentrations, and when available, SOA O:C and thermodynamic-based volatility data. The SOM-TOMAS model will be used with those parameters to perform atmospherically relevant (i.e., lower seed and OH concentrations, no vapor wall losses) simulations to study the evolution of SOA mass yields and composition over several days. Sensitivity simulations will be performed to systematically investigate the role of aging, NO_x , and phase state. Finally, those simulations will be used to develop updated volatility basis set fits for use in atmospheric models.

3AC.6

Constraining the Impact of Microorganisms on Atmospheric Aerosol and Cloud Chemistry. ALISON FANKHAUSER, Dexter D. Antonio, Asher M. Krell, Simone J. Alston, Scott Banta, V. Faye McNeill, *Columbia University*

We use a modeling approach to evaluate the potential impact of microbial metabolism on the organic composition of cloud droplets and atmospheric aerosols. Microbial consumption rates for small organic molecules typically found in cloud and aerosol water were incorporated in to a 0-D multiphase photochemical atmospheric chemistry model. We then use the model to simulate the evolution of the organic content of individual cloud and aerosol particles, along with the atmospheric gas phase, under typical conditions. We find that metabolically active microorganisms may significantly impact the composition of the individual aerosols and cloud droplets in which they reside. However, due to the low density of metabolically active cells in the atmosphere, the impact of these processes on the chemical composition of the overall population of cloud droplets of aerosols, or on gas phase chemistry, is likely negligible.

3AD.1

Computational Modeling of Multispecies Evolving Aerosol Delivery in the Human Respiratory Tract. FRANCESCO LUCCI, Mahdi Asgari, Edo Frederix, Arkadiusz Kuczaj, *Philip Morris International R&D*

Numerous experimental and computational approaches have been developed to understand aerosol inhalation processes targeting various types of aerosols (e.g., solid particles). Transport and deposition of evolving aerosols generated from chemical mixtures are particularly challenging due to complexities arising from the interplay of physics and chemistry properties driven together by the airflow thermodynamics. These processes govern both the gas-liquid phase partitioning of mixture constituents and particle size distribution properties, eventually impacting aerosol delivery and deposition. To investigate aerosols generated from multispecies complex mixtures in particular, we have developed the open-source computational fluid dynamics code AeroSolved (www.aerosolved.com), in which aerosol nucleation, condensation/evaporation, and coagulation processes can be investigated within a density-coupled framework. This gives a unique capability to study the flows in the human respiratory tract in detail, with particular attention to aerosol evolution and deposition by diffusion, sedimentation, and impaction. Following our recent work concerning multispecies aerosol evolution and deposition in a bent pipe (Asgari et al., JAS (129), 2019), we extended its scope to simulate liquid particle (consisting of propylene glycol, glycerol, and water) flows in a respiratory tract geometry up to six generations of the tracheobronchial tree. Our computational models were validated by comparing with the available literature data for aerosol evolution and deposition under controlled experimental conditions. We considered air flow rates ranging from 1.5 to 30 L/min as equivalent to puffing and inhalation flow rates, including steady and transitional flows. Our results showed that particle size evolution can significantly influence the deposition efficiency favoring or inhibiting the inertial and diffusional deposition mechanisms. We also showed that species-specific deposited liquid mass is also changed remarkably due to particle evolution. We present a comprehensive set of simulation scenarios and learnings concerning complex mixture aerosol behavior during the inhalation process and relevant for the dosimetry purposes.

3AD.2

Profiling Sources and Chemical Aging Effects on the Oxidative Potential of Organic Aerosol. SHUNYAO WANG, Karl Demmans, Jianjun Han, Manpreet Takhar, Zeng Rui, Peng Hui, Arthur W. H. Chan, *University of Toronto*

Exposure to ambient particles is associated with numerous adverse health outcomes. However, due to the complex properties and dynamic evolution of organic aerosol (OA), its ability to cause oxidative stress (oxidative potential, or OP) and the corresponding adverse health outcomes remain poorly understood. Unlike the other indirect cellular and acellular OP measurements, electron paramagnetic resonance (EPR) can directly delineate the type and quantity of free radical species. As the least ambiguous method for free radical measurements, different spin trap techniques were applied to the EPR OP measurement. In this work, a direct free radical profile (types, abundances and their lifetimes) was derived for OA emerged from various sources. In addition to secondary organic aerosol (SOA) from specific biogenic and anthropogenic hydrocarbon precursors, high radical signals were found in cooking and wood-burning emissions, indicating the potential health impact from indoor cooking activity and wildfire events. Using naphthalene SOA (NSOA) as a model system, relative abundances of reactive oxygen species in aerosol evolved under various photochemical aging processes were compared and linked to the varied chemical composition measured by mass spectrometry. Within a single type of OA system, the EPR measured OP trend along with atmospheric aging processes was found to be consistent with OP results from other acellular and cellular measurements. Mixing effects of different OA compositions on the free radical production were also investigated. Our study provides insights into how the chemical composition and atmospheric formation process of ambient particles are related with its ability to cause oxidative stress and potential adverse health outcomes.

3AD.3

Oxidative Potential of PM_{2.5} Semi-volatile Species in an Urban Atmosphere. MILAD PIRHADI, Amirhosein Mousavi, Sina Taghvaei, Mohammad Sowlat, Constantinos Sioutas, *University of Southern California*

In this study, we investigated the physicochemical characteristics and oxidative potential of the semi-volatile components of the ambient particulate matter (PM). The versatile aerosol concentration enrichment system (VACES) was used to collect concentrated ambient and thermodenuded fine particulate matter (PM_{2.5}) concurrently, at an urban site located in the central Los Angeles during summer 2018 and winter 2019. We used a thermodenuder to selectively remove the semi-volatile components of the concentrated PM_{2.5} at the 45-50 and 95-100 °C. The oxidative potential of the collected samples was quantified by means of an in-vitro cell-based alveolar macrophage (AM) assay. The volatility profile of the various PM_{2.5} components and corresponding effect on oxidative potential was quantified by conducting chemical analysis on the collected samples including elemental and organic carbon, inorganic ions, water soluble organic carbon (WSOC), metals, and polycyclic aromatic hydrocarbons (PAHs). While the refractory PM constituents including elemental carbon and metals were slightly affected by the heating, the labile components of PM_{2.5} such as PAHs and organic carbon illustrated progressive concentration losses with increase in the thermodenuder temperature. Significant reductions in the PM_{2.5} oxidative potential were observed as the semi-volatile components of the PM_{2.5} were removed. While the losses were 45% and 74% at the 50 and 100 °C, respectively, in the summer period, the corresponding losses at the winter campaign were 56% and 85%, respectively. Therefore, the semi-volatile components are responsible for a significant fraction of the PM_{2.5} oxidative potential. Furthermore, the results of the regression analysis illustrated a strong association between the PM_{2.5} oxidative potential and organic carbon (OC), water soluble organic carbon (WSOC) and PAHs in both summer and winter periods.

3AD.4

The Impact of Cooking Aerosol on Human Brain and Heart. MEHDI AMOUEI TORKMAHALLEH, Motahareh Naser, Zhibek Bekezhanqyzy, Aidana Gimnkan, Nurzhan Sholpan, Raikhangul Gabdrashova, Milad Malekipirbazari, Mojtaba Jozizade, Mahsa Tabesh, Hamta Farrokhi, Reza Khanbabaie, Hossein Mehri-Dehnavi, *Chemical and Aerosol Research Team, Nazarbayev University*

The cooking emission in residential or commercial kitchens is one of the main indoor PM sources that results in human exposure to high concentrations of ultrafine particles (UFPs). While there are few clinical studies investigating the cardiovascular effects of cooking aerosol, no clinical study exists in the literature investigating the impact of cooking aerosol on human brain. The main objective of this study was to investigate the blood pressure, heart rate and brain's wave pattern changes during and after acute exposure to cooking aerosol. Twelve volunteers were monitored for brain wave pattern and 60 volunteers were examined for blood pressure (BP) and heart rate (HR). All volunteers were non-atopic, non-smoking, and healthy adults (18-46 years old). The measurements were conducted before, end of, and 30 minutes after cooking, using electroencephalography (EEG) and up to 2 hours after cooking for BP and HR. Frying ground beef in some sunflower oil using electric stove representing a low emission recipe was conducted. UFPs, particulate matter (PM₁, PM_{2.5}, PM₄, PM₁₀), CO₂, indoor temperature, indoor RH, oil and meat temperatures were monitored continuously throughout the experiments. It was found that Systolic blood pressure (SBP) statistically significantly increased due to exposure to cooking aerosol while no change was observed in Diastolic blood pressure (DBP) and HR. Furthermore, cooking aerosol significantly increased Beta and alpha band of the brain while delta band significantly decreased. All changes occurred on frontal and temporal lobes of the brain. Both cardiovascular and nervous impacts due to exposure to cooking aerosol was observed mainly with a delay up to 2 hours post-exposure. Comparisons between this study and the EEG pattern of those who were exposed to diesel engine exhaust and smoking fumes as well as neurodegenerative diseases such as Alzheimer and Parkinson will be presented.

3AD.5

Chronic Exposure to Real-time Traffic Related Air Pollution Increases Neuroinflammation and Exacerbates Plaque Burden in TgF344-AD Rats. Kelley Patten, Anthony Valenzuela, Ameer Taha, Keith Bein, ANTHONY S. WEXLER, Pamela Lein, *University of California, Davis*

Introduction. Epidemiological studies have linked traffic-related air pollution (TRAP) to increased risk of Alzheimer's disease (AD). However, this association has yet to be confirmed in a preclinical model. Moreover, the mechanism(s) by which TRAP influences AD are unclear.

Methods. To address these issues, we exposed male and female TgF344-AD rats and congenic controls to real-time TRAP or filtered air (FA) over the course of 15 months, using a mobile exposure facility that samples air from a highway tunnel in the Bay Area of California. Rats were exposed to TRAP or FA from postnatal day 28 to 15 months of age. At 3, 6, 10, and 15 months of age, brain samples were collected, and analyzed for plaque burden, bioactive lipids, microgliosis, astrogliosis, and cytokine protein levels.

Conclusions. Chronic TRAP exposure increased plaque burden in AD transgenic rats at 6 months. In addition, we found that TRAP exposure increased pro-inflammatory cytokines as early as 3 months of age, and modulated levels of both pro- and anti-inflammatory cytokines at later time points. Finally, both microgliosis and astrogliosis were increased by TRAP exposure. These data suggest that TRAP may exacerbate AD-relevant phenotypes, and that these results may be mediated through neuroinflammation.

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3AD.6

Temporal Changes in the Per Unit Mass Toxicity of Ambient PM2.5 in New York State. PHILIP K. HOPKE, Daniel Croft, Wangjian Zhang, Shao Lin, Mauro Masiol, Stefania Squizzato, Sally Thurston, Edwin van Wijngaaten, Mark Utell, David Q. Rich, *University of Rochester Medical Center*

From 2005 to 2016, there have been dramatic decreases in PM2.5 and the primary pollutant gases across New York State as a result of regulatory actions and changing economic conditions. The major PM constituents that declined include sulfate, nitrate, elemental carbon (EC), and primary organic carbon (POC). However, ozone and secondary organic aerosol (SOA) have increased in many locations. Source apportionment allows identification of the trends in source-specific PM. Secondary inorganic aerosol types have decreased, but spark-ignition vehicular contributions have increased. Rates of cardiopulmonary and respiratory infectious hospitalizations and emergency department (ED) visits in Buffalo, Rochester, Albany, and New York City over this period have also declined. However, an examination of these associations in 3 time intervals, 2005-07, 2008-13, and 2014-16, showed that for some health outcomes, the excess rates of hospitalization and/or ED visits per unit mass of PM2.5 have increased. When assessing associations between these hospitalization and ED visits and source-specific PM2.5, the apparent change in PM2.5 toxicity is associated with the changing relative proportions of the various source contributions over these time intervals. These results will be presented, and their implications for future regulatory actions to further improve public health, will be discussed.

3BC.1

Pregnant Women's Exposure to Household Air Pollution during a LPG Cookstove Intervention in Rural Bangladesh: The Value of Real-Time Data. Maggie Abbott, JONATHAN THORNBURG, Sajia Islam, Masum Billah, Fariha Tasnim, Seung-Hyun Cho, Ashraf Alam, Camille Raynes-Greenow, *RTI International*

We developed a protocol for a cluster randomised controlled trial to assess the impact of liquid petroleum gas (LPG) cooking compared to usual cooking on perinatal mortality in pregnant women in rural Bangladesh (ACTRN12618001214224). As part of the protocol, we assessed the value of personal monitoring to measure reductions in household air pollution exposure before and after the intervention.

We measured PM_{2.5} exposure with the MicroPEM. Gravimetric and optical density analyses provided total mass and black carbon mass concentrations, respectively. MicroPEM nephelometer data provided temporal insights into the participants' exposure. We enrolled 30 pregnant women for 24-hours of exposure assessment when following traditional cooking practices (baseline) and repeated after receiving their LPG cookstove (intervention).

We collected valid baseline-intervention MicroPEM data from 22 of the 30 women. Participants wore the MicroPEM 77% and 69% of the time during baseline and intervention. Mean gravimetric PM_{2.5} concentrations during baseline and intervention were similar: 81.3 µg/m³ vs. 75.3 µg/m³. BC was also similar: 56.4 µg/m³ vs. 68.7 µg/m³. A temporal pattern in PM_{2.5} concentrations indicated PM_{2.5} exposure was lower when cooking with the LPG stove. The mean MicroPEM nephelometer concentration during cooking periods with LPG was 84.6 µg/m³ vs. 136.5 µg/m³ with traditional stoves (p<0.0001).

External factors to the LPG cookstove intervention influenced the time-integrated PM_{2.5} concentrations. Baseline measurements occurred in May-June, monsoon season in Bangladesh. The LPG intervention occurred in November, a dry month with widespread agricultural activities. The consistent rain during the monsoon lowered ambient PM_{2.5} whereas crop harvest increased ambient PM_{2.5}. These factors elevated the background PM_{2.5} exposures during the intervention that are not associated with the LPG cookstove. In complex air pollution environments, real-time PM_{2.5} exposure data will help evaluate the effectiveness of a clean-cooking intervention.

3BC.2

Linking Cookstove Emissions to Indoor Air Quality: Outcome of a Multi-year 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, an acknowledged threat to human health. In this study, we assess indoor PM_{2.5} and its variability during a cookstove intervention trial in which multiple stoves were offered to households in two rural areas in India (Kullu in Himachal Pradesh; Koppal in Karnataka). We also aim to improve links between estimates of cookstove emissions and indoor PM_{2.5}. The study had three ~3-month-long measurement periods (baseline, follow-up-1, follow-up-2) in each location. We measured real-time and gravimetric indoor PM_{2.5} concentrations during ~5000 cooking events of traditional and alternate biomass and modern-fuel stoves. We also conducted simultaneous emission measurements for a subset of those cooking events.

Intention-to-treat analysis in Koppal showed significant reduction in indoor PM_{2.5} in intervention households relative to control households only in follow-up-1, indicating mixed effectiveness. Black carbon concentrations showed significantly different distributions in different seasons. In general, Kullu households had ~50% lower PM_{2.5} concentration than Koppal, strong evidence of inter-site variability in PM_{2.5}. Higher estimated air exchange rate (AER; 11±5 h⁻¹) and lower cooking time (3.6±2.9 h) in Kullu households compared to Koppal (7±4 h⁻¹ and 5.3±3.0 h) may explain the reduced PM_{2.5} concentration in Kullu. Households in Kullu and Koppal having LPG had median PM_{2.5} concentrations of 91 and 111 µg/m³ respectively, 1.5-2 times lower than households without LPG. In Koppal, PM_{2.5} concentrations were 1.5-2.5 times higher in households without chimneys than those with chimneys. We will apply mixed effect modeling using seasons, locations, AER, household ventilation characteristics (e.g. presence of chimney, doors and windows), stove types, fuel use, and presence of other emission sources (e.g. incense, lamp) as predictors to identify the factors contributing to indoor PM_{2.5} variability. Finally, we will develop a statistical model linking measured emissions rates and PM_{2.5} concentrations.

3BC.3

Initial Evaluation of a Heating Stove Changeout Program in the Navajo Nation Featuring a Culturally-Appropriate Wood/Coal Stove. Naomi Chang, Tennille Denetdeel, Jeri Garfield, Sky Izzo, Michael King, Chris Yazzie, Mark Bauer, Paul Solomon, Kathleen Stewart, LUPITA MONTOYA, *University of Colorado Boulder*

Many Navajo households rely on wood and coal for residential heating, using old, inefficient, and polluting heating stoves. A study by Bunnell et al. (2010) reported higher rates of hospitalization due to respiratory conditions during the winter relative to summer in the Shiprock Chapter, likely due to these heating practices. Using a new framework that integrated community perception, culture, and science, Champion et al. (2017) determined that the most effective and culturally-appropriate heating option for this community would be a new dual-fuel (wood/coal) heating stove. Such “Navajo Stove” was subsequently designed, USEPA-certified, and included in a stove changeout program taking place in portions of the Navajo Nation. The stove changeout program – with \$4.7 million in funding – started in 2018 and will occur over 5 years in seven Chapters of the Navajo Nation, including Shiprock. Households with elders, children, veterans, and people with respiratory and cardiovascular health conditions are prioritized.

A research study was designed to assess changes in indoor air quality and respiratory health symptoms of participants in this stove changeout program. To participate in the research study, households requesting a Navajo Stove were recruited through referrals from program coordinators. A First Pilot Study was conducted during the heating season (March-April) of 2018 in Shiprock, NM. Initial results of this Pilot Study, as well as results of a correction factor study for wood/coal smoke will be presented.

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3BC.4 (INVITED)

Improving Smoke Exposure Assessment for Surveillance and Epidemiology in British Columbia, Canada. SARAH HENDERSON, *British Columbia Centre for Disease Control*

Smoke from biomass burning is one of the most important sources of air pollution in the Canadian province of British Columbia (BC). In winter, many coastal, northern, and alpine communities are affected by emissions from residential wood-burning appliances. In summer, annual wildfire activity leads to more extreme and unpredictable smoke exposures across the entire province and beyond. More recently, the unprecedented 2017 and 2018 wildfire seasons lasted for several weeks and blanketed most of western Canada in smoke for extended periods.

While emissions from other sources such as traffic and industry have been decreasing in BC, emissions from residential wood-burning and wildfire smoke have been increasing over the past decade. This reality makes it critically important for the public health sector to understand the short- and long-term impacts of biomass smoke exposures. The BC Centre for Disease Control (BCCDC) has been developing a range of tools to assess these smoke exposures and their effects on the health of different populations.

Mobile monitoring in communities affected by residential woodsmoke allows for detailed mapping of the air quality impacts. While such campaigns can be expensive and time-consuming for specific research groups to undertake, citizen scientists are often willing to do the work with guidance and support from more experienced investigators. The first part of this talk will cover tools that the BCCDC has developed for citizen science mapping of residential woodsmoke exposures.

Wildfire smoke pollution is dynamic in both space and time, making it challenging to understand exposures based solely on the data from regulatory monitoring networks. The Optimized Statistical Smoke Exposure Model (OSSEM) integrates data from multiple remote sensing sources to map 1-hour smoke exposures across BC. The second part of this talk will cover the relationship between OSSEM estimates and cardiorespiratory ambulance dispatches.

3BC.5

Implications of Photochemical Ageing for Toxicity and Source Apportionment of Wood Combustion Aerosols: A Combined Biological and Chemical Study. Hendryk Czech, Toni Miersch, Anni Hartikainen, Mika Ihalainen, Sebastiano di Bucchianico, Jürgen Orasche, Sebastian Oeder, Jarkko Tissari, Thorsten Streibel, Jürgen Schnelle-Kreis, Pasi Javala, Maija-Riitta Hirvonen, Olli Sippula, Jorma Jokiniemi, RALF ZIMMERMANN, and further members of the HICE consortium, *University of Rostock and Helmholtz Zentrum Munich, Germany*

Wood combustion in residential stoves is a substantial contributor to air pollution and releases high levels of particle-bound polycyclic aromatic hydrocarbons (PAH) and oxygenated PAH (OPAH). In the atmosphere those compounds undergo chemical transformation along with SOA formation from gaseous compounds, which is changing the toxicity of the wood combustion emissions. In this study, we aged spruce-logwood combustion-aerosol by a recently described high-flow oxidation flow-tube reactor (Ihalainen et al., AS&T, 2019) and investigated the effect of ageing on PAH and OPAH emissions, PAH diagnostic ratios for emission source identification and the carcinogenicity (based on PAH toxicity equivalent approach (PAH-TEQ)). The cytotoxicity and genotoxicity of primary and aged emissions were assessed in 4 h in vitro air-liquid-interface (ALI) exposures of human lung cell lines (A549, BEAS2B). Furthermore, transcriptome and proteome analysis of the exposed cells and controls were performed (multi-omics approach, Oeder et al., PLoS one, 2015). The combustion of spruce logwood released 404 μg /330 μg MJ⁻¹ of analysed OPAH, most of which are known or potential mutagens/carcinogens. Photochemical flow-tube processing substantially degraded particle-bound PAH (PAH-TEQ declines by 45-80% per equivalent day of photochemical-ageing). Compared to PAH, OPAH were less affected, while hydroxylated-PAH increased by secondary formation. Genotoxicity is increased significantly from clean air control to both, primary and aged aerosol (comet assay), but without quantitative differences between primary and aged spruce aerosol, despite the drastically reduced genotoxic PAH-concentrations. This study also showed an increased cytotoxicity of wood combustion emission by photochemical atmospheric transformation. The in-depth transcriptome analysis revealed different genotoxic mechanisms and induced DNA damage. Some diagnostic PAH ratios to identify wood combustion emissions in ambient air remain stable during photochemical ageing while other ratios allow monitoring of the photochemical age.

3CC.1

Measuring and Modeling the Water-Solubility Distribution of Organic Aerosol. SHUNSUKE NAKAO, Vikram Pratap, Aditya Kiran Srikakulapu, *Clarkson University*

The water-solubility of organics is a key parameter that may determine the hygroscopic growth of aerosol, cloud droplet activation, and liquid-liquid phase separation (LLPS). However, direct measurements of water-solubility are limited. Previous approaches to characterization of the solubility of OA includes extraction with multiple solvents with different polarity as well as activation of cloud condensation nuclei (CCN) with varying inorganic seed fraction. However, such approaches are labor intensive and only allow classification of water solubility into a few levels. This study developed a new experimental approach for characterizing the continuum of solubility distribution in OA based on the combination of high-performance liquid chromatography (HPLC) and charged aerosol detection (CAD). Unlike the conventional detection methods used in HPLC, such as UV-visible absorption or mass spectrometry, aerosol measurements allow quantification of analytes irrespective of chemical properties. The method was validated using a series of standard compounds showing a strong correlation between the HPLC retention time and estimated water-solubility. Semi-volatile compounds with saturation concentration above $\sim 1\mu\text{g m}^{-3}$ were observed to significantly evaporate in the experimental setup; therefore, caution must be taken in interpreting the solubility distribution of semi-volatile OA. The method was applied to the characterization of secondary organic aerosol (SOA) produced from the ozonolysis of α -pinene. The results indicate that solubility of α -pinene SOA components varies by six orders of magnitude. The implication of the wide solubility distribution to cloud droplet activation was evaluated using the Köhler theory. It was estimated that approximately 10-40% of α -pinene SOA components remain undissolved at the point of droplet activation when the volume fraction of inorganic components in aerosol is varied from 0 to 50%. Molecular identities of the low-solubility compounds remain unknown. Implications of the polarity distribution on LLPS and the gap in sub-saturated and super-saturated aerosol hygroscopicity will be discussed.

3CC.2

Impact of Improved Representation of Aerosol Mixing State on Air-Quality-Weather Interactions. ROBIN STEVENS, Ashu Dastoor, *Environment and Climate Change Canada*

Aerosol chemical mixing-state, or the degree to which aerosol is internally- or externally-mixed, is important for both aerosol hygroscopic and radiative properties (Riemer et al. 2019; Stevens et al. 2019). Internal mixing of hydrophilic and hydrophobic species can allow the hydrophobic species to act as cloud condensation nuclei and to be more-efficiently removed by wet deposition. When internally-mixed, weakly-absorbing species act a lens on strongly-absorbing species (e.g. black carbon). This enhances absorption, compared to the case where the weakly- and strongly-absorbing species are externally-mixed. In the real atmosphere, aerosol is neither fully-externally-mixed nor fully-internally-mixed.

We implement a more-detailed representation of the aerosol mixing-state in the GEM-MACH air quality model with online air-quality-weather interactions. Our approach was inspired by MOSAIC-MIX (Ching et al. 2016): We independently account for both changes in hygroscopicity and black carbon mass fraction, as aerosol hygroscopic properties and radiative properties do not necessarily co-vary. The air-quality-weather interactions in GEM-MACH include aerosol-radiation interactions and changes in cloud droplet activation based on cloud condensation nuclei concentrations. We perform a case study focused on biomass-burning over North America to evaluate the results with the new representation of aerosol mixing state, both against the original size-resolved internally-mixed assumption and against observations. We investigate the interactions between the representation of aerosol mixing state and air-quality-weather interactions.

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3CC.3

Evaluating the Impacts of In-Cloud Chemistry on Resuspended Aerosol Particles after Cloud Evaporation using a Particle Resolved Model. YU YAO, Nicole Riemer, Matt Dawson, *University of Illinois at Urbana-Champaign*

Aerosol particle size distributions undergo physical and chemical changes during cloud processing. After cloud evaporation, the released particles can have different activation potentials than the particles before cloud processing because of changes in size and chemical composition. Current models use simplified assumptions about these mass and size changes due to cloud processing. For example, the aerosol module coupled to WRF-Chem assumes the cloud-borne aerosol mass is proportional to cloud droplet mass, and in the Community Multiscale Air Quality Modeling System (CMAQ), it is assumed that the mass formed by aqueous phase chemistry is added to the accumulation mode aerosol. In real environments, particles with different composition and size experience different net effects from aqueous chemical processing, so the impact of in-cloud chemistry on the resuspended aerosol size distribution can be more complicated.

In this study, we focus on the resuspension of aerosol populations, and the changes of aerosol microphysical properties after cloud evaporation. We simulated several urban plume scenarios that produced populations with a wide variety of 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, at various cooling rates. The aqueous chemistry mechanism coupled to 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 and sizes of individual aerosol particles without averaging their composition within size bins or modes. We will quantify the species mass and particle size differences of the aerosol population before and after cloud processing, and relative changes to critical supersaturations will be used to evaluate the microphysical changes.

3CC.4

Effects of GHG Mitigation Strategies in Future Climate over California. ANIKENDER KUMAR, Michael Kleeman, Christina Zapata, *University of California, Davis*

California has committed to reduce greenhouse gas (GHG) emissions by 80% relative to 1990 levels by the year 2050. This effort will require adoption of low-carbon energy sources across all economic sectors, transforming the airborne particulate matter in California's atmosphere at the same time that it reduces GHG emissions. In this study, we examine the effects of changing PM composition on radiative forcing under two energy scenarios: business-as-usual (BAU) and low-carbon energy scenario (GHG-Step). Calculations are performed using the source-oriented WRF/Chem (SOWC) model, which can track a six dimensional aerosol variable (X, Z, Y, Size bin, Source type, Species) through explicit simulations of atmospheric chemistry and physics. This approach allows particles with the same size from different sources to age into different chemical compositions that depend on the chemical and hygroscopic properties of the primary seed particles.

The BAU and GHG-Step statewide future emission scenarios were constructed using the energy-economic optimization model, CA-TIMES. The SOWC model is applied for the year 2054 with 12 km resolution over California. Meteorological initial and boundary conditions are updated using Community Earth System Model (CESM) model with Representative Concentration Pathway (RCP8.5) future scenario. Surface temperature, precipitation, and top of the atmosphere (TOA) forcing will be compared in the BAU and GHG-Step scenarios. Implications for future climate in California will be discussed.

3CC.5

Stratocumulus Cloud-top Inhomogeneous Entrainment Parcel Model Parameterization. KEVIN SANCHEZ, Greg Roberts, Minghui Diao, Lynn Russell, *Scripps Institution of Oceanography*

Observations of stratocumulus clouds from the Southern Ocean Clouds, Radiation, Aerosol Transport Experimental Study (SOCRATES) were used to quantify the effect of cloud-top entrainment on the shortwave cloud radiative forcing (SWCF). Marine stratocumulus clouds are an important part of the global heat budget because of their large horizontal extent. However, their radiative forcing is highly uncertain due to sensitivity of their radiative properties to slight variations in cloud microphysical properties. The marine boundary layer also has few sources of cloud condensation nuclei, especially in the Southern Ocean, adding to the uncertainty. A cloud parcel model was utilized to simulate the observed cloud profiles. A mixing line entrainment parameterization, first shown by Sanchez et al. 2017, is applied to the simulations to account for cloud droplet evaporation due to cloud-top entrainment of warm, dry free tropospheric air, improving closure of cloud droplet number concentrations (CDNC) and SWCF. The mixing line parameterization uses thermodynamically conserved variables, derived from measured state parameters, to identify mixing of air into the cloud-top. Previously this entrainment parameterization has been applied to marine stratocumulus clouds on the west coast of Ireland and over Cyprus and compared to in-cloud vertical profiles of solar irradiance and cloud droplet extinction. In this study the parameterization is compared directly to measured CDNC profiles. Results indicate cloud-top entrainment decreases the SWCF between 37 and 85 W m⁻² and CDNC between 35% and 60% for the five cases in this study. In addition, simulations with varying updraft velocities and below cloud particle concentrations indicate the CDNC and SWCF are significantly more sensitive to drying from cloud-top entrainment than changes in updraft velocity and particle concentrations, emphasizing the importance of accurately accounting for cloud-top entrainment.

3CC.6

Surface Aerosol Bimodality Due to Continental Cloud Processing and Photochemical Particle Production. JAMES HUDSON, Stephen Noble, *Desert Research Institute*

Relationships between clouds and surface aerosol were investigated at the Oklahoma ARM site. Cloud chemical transformations, coalescence, and Brownian capture increase material within cloud droplets. Then when droplets evaporate their residuals are larger than un-nucleated particles. Bimodal aerosol is thus created by moving Aitken particles to the accumulation mode. Clouds also block solar radiation that causes photochemical production of small particles that grow into the Aitken mode. Highly significant positive correlations of remotely-sensed cloud fractions (cf) with time-lagged Aitken and accumulation mode mean particle diameters (mpd) isolated the effects of cloud processing on both modes. Positive correlations of cf with accumulation concentrations and negative correlations of cf with Aitken concentrations provided further evidence of cloud processing. Photochemical production under clear daylight skies worked together with cloud processing to further enhance Aitken mpd and concentration correlations with cf. Cloud-processed aerosol was evident only during daylight and only when the boundary layer mixing height exceeded cloud base altitude. Greater cf, especially consecutive high cf hours increased accumulation and Aitken mpd and accumulation concentrations while it decreased Aitken concentrations. Lower cf, especially consecutive hours of no clouds, decreased overall mpd and did not enhance the accumulation mode. These results implicated clouds as the source of the accumulation mode. Thus, clouds explained bimodal aerosol over the mid North American continent.

Unlike previous bimodal aerosol observations, the degree of bimodality here is directly linked to the extent of cloudiness to thus better substantiate that cloud processing is the source of the accumulation mode. Augmentation of the accumulation mode was absent when there were few clouds or no clouds. The fact that Aitken particles nucleated cloud droplets in the presence of high accumulation particle concentrations indicated high cloud supersaturations in continental air. This indicates that CCN are not confined to the accumulation mode.

3IM.1

Temperature Dependent Phase Study of Aerosols Using Droplet Microfluidics. PRIYATANU ROY, Cari Dutcher, *University of Minnesota*

Atmospheric aerosols containing multiple organic and inorganic components experience a broad range of relative humidities and temperatures which govern their phase state. Many aerosol properties including particle morphology, hygroscopicity, surface tension, viscosity, optical cross section and equilibrium partitioning are influenced by their phase state. In situ observation of factors including relative humidity and temperature on single aerosol droplets are difficult, whereas laboratory measurements using droplet microfluidics are both simple and cost-effective. In this work, microfluidic devices are used to generate and study phase states of aqueous droplets containing sea spray aerosol samples and chemical mimics using both static trap and flow-through approaches at temperatures as low as -40°C. The static trap device dehydrates trapped droplets in a quasi-equilibrium method to study the effect of relative humidity and water loss on liquid-liquid phase separation and crystallization at different subcooled temperatures inside a temperature-controlled cell utilizing liquid nitrogen cooling and resistive heating. Preliminary results show low temperatures do affect the phase separation behavior depending on the composition and solute ratios of the droplet. The high-throughput flow-through device measures ice nucleation temperature of droplets using on-chip platinum resistive temperature sensors and sits on top of a temperature control block with seven discrete temperature zones using Peltier elements which use the liquid nitrogen cooled temperature-controlled cell as a heat sink. The measurements will be used to predict the cloud and ice formation activity of both land-based and sea spray aerosols.

3IM.2

A New Approach for in Situ Picolitre Sampling of Aerosol Using Optically Trapped Droplets. MALCOLM KITTLE, Rachael E.H. Miles, Jason Murrell, Rebecca Hopkins, Jonathan P. Reid, *University of Bristol*

In the event of a Chemical Warfare Agent (CWA) release, it is anticipated that CWA would be present in the atmosphere as vapour and/or aerosol. A sensing capability must provide a fast, high confidence response with low false alarms to background aerosols commonly encountered in operational environments. In addition, the technique should allow detection of a broad range of hazards, and be able to sample and analyse both gas phase species and condensed phase particles (typically >100 nm in diameter).

A novel instrument has been designed that uses a single optically trapped droplet of sub-picolitre volume as an ultrasensitive sampler of gas phase or aerosol composition, with potential applicability to CWA detection. Vapour or aerosol present in the surrounding environment is sampled through mass transfer into the probe droplet. This uptake produces a change in the probe droplet size and composition, which can be characterised by monitoring the evolution of the probe droplet's Raman spectrum. New spontaneous Raman bands emerge as chemicals are partitioned into the tweezed droplet, allowing composition of the sampled mass to be determined. Further, the radius and refractive index of the droplet confined in the optical trap can be determined from the whispering gallery modes in the simulated Raman spectrum via Mie theory.

As a proof-of-concept, a constant output atomiser is used to generate aerosol from sodium chloride and sodium citrate. The mass concentration and size distribution of aerosol particles flowing into the trapping cell are measured by a nanoparticle sizer. Raman spectroscopy is then used to characterise the change in size and composition of the probe droplet. Use of these combined techniques allows the relationship between aerosol mass concentration and mass uptake by the trapped droplet to be investigated, ultimately providing an understanding of aerosol accretion rates and instrument sensitivity of this novel approach.

3IM.3

Laser-induced Incandescence: Need to Revisit. IGOR ALTMAN, Fengshan Liu, *Naval Air Warfare Center Weapons Division, USA*

Laser-induced incandescence (LII) is currently being considered a powerful tool for characterization of the condensed phase in combustion diagnostics of two-phase systems [1]. The interpretation of LII experiment is based on two main postulated statements: the light emission from the laser irradiated particles is related to the Planck blackbody radiation, as a result of particle temperature rise by laser energy absorption, and the particle heat transfer to the environment determines the emission decay after the laser pulse. These two statements seem so obvious that, in our knowledge, have never been deeply analyzed except the old attempt to challenge the LII fundamentals [2].

Recently, LII practitioners have faced a couple of issues [3] that they could not resolve based on the existing LII theory [4]. They found that the laser energy in the experiment is not enough to heat the particle up to a temperature, at which it can emit a detectable LII signal, and the energy deficit far exceeds 10 at some conditions. Besides the unexplained issues, LII predictions of the energy accommodation coefficient in the range of 0.1-1 need to be challenged as well [5, 6]. Then, there seems more than enough evidence to introduce some alternative LII scenario.

The essence of our explanation of the LII occurrence is the thermal isolation between the systems of electrons and phonons in the laser irradiated particles during and after the laser pulse, whose possible mechanism is described in [7]. Based on this thermal isolation we are able to reconcile all major LII issues. The LII scenario we introduce does necessarily lead to the need to revisit the LII results in their entirety.

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3IM.4

Aerosol Mass Spectrometer for On-Line Detection of Polycyclic Hydrocarbons as Well as Inorganic Cations and Anions from Single Particles. RALF ZIMMERMANN, Julian Schade, Robert Irsig, Martin Sklorz, Johannes Passig, *Helmholtz Zentrum München and University of Rostock*

Inhalation of Polycyclic Aromatic Hydrocarbons (PAHs) is a well-known cause of morbidity and mortality. Furthermore, PAHs play an important role in the climate system because of their specific optical properties and effects on the formation of secondary organic aerosols. However, data on their distribution in aerosols are limited. This is of particular concern since details about their mixing state are crucial to assess health effects. For example, PAHs may be equally distributed over the ensemble or could be concentrated within a specific sub-population, inducing local effects upon particle-in-lung deposition and potential cancer development. Consequently, novel on-line techniques addressing PAHs on a single-particle scale while providing source information are desired.

Our approach is based on Single Particle Mass Spectrometry. Herein, particles are introduced into vacuum and sized via laser velocimetry. Prior to ionization, organics are desorbed by an IR-pulse. Key idea of our method is a spatially formed ionization laser profile that facilitates simultaneous Resonance-Enhanced Multi-Photon Ionization (REMPI) of the desorbed plume and Laser Desorption/Ionization (LDI) of the residual with one single UV-pulse. Thus, we introduce a route to obtain the full LDI-information of both positive and negative inorganic ions for source apportionment combined with health-relevant PAHs via REMPI.

In contrast to previously reported methods, cations and anions from LDI can now be detected, together with fully-fledged PAH-spectra from REMPI. Because all ions are formed within one combined ionization step, no further laser beyond the two sources for conventional two-step approaches is required. The method allows detailed insight into the mixing state of PAHs on different particle types. First on-line experiments on combustion aerosols demonstrate the methods capabilities to unravel the distribution of health-critical PAHs in the particle phase in real time.

3IM.5

Chemical Reactions on Optically Trapped Single Particles. CHUJI WANG, Zhiyong Gong, Gorden Videen, Yong-Le Pan, *Mississippi State University*

Single-particle study is an emerging research topic in aerosol science and engineering, which is made possible by recent developments in optical trapping and manipulation techniques. From optical tweezers, the early approach which uses a single tightly focused laser beam to levitate and trap non-absorbing micron-sized particles, to the recently developed optical traps such as the universal optical trap (UOT) that can trap particles of arbitrary chemical and physical properties in different media, optical trapping finds its new applications in aerosol. When a particle is optically levitated in air, it is free from chemical and physical surface interference as well as electrical charge. To date, a wide variety of single particles including carbons, dusts, metal oxides, pollens, spores, organic/inorganic droplets, etc. have been characterized using cavity ringdown spectroscopy, Raman spectroscopy, light scattering, imaging, and or laser-induced fluorescence. As single particles can be trapped stably in the UOT for a long period of time, temporal evolution on chemical and physical properties of trapped particles can also be studied. Very recently, we have demonstrated that we can use a trapped particle as a micro-reactor to study chemical reactions. We report our latest efforts and progresses in this new adventure.

3IM.6

A Single Particle Approach for Exploring Aerosol Photochemistry and Optical Properties. JAMES F. DAVIES, Chelsea Price, Alison Bain, Thomas Preston, *University of California, Riverside*

A coupled understanding of the evolving chemical composition and related physical and optical characteristics of aerosol in the atmosphere is required to accurately predict their role in the environment. Aerosol become chemically transformed by several processes, such as evaporation and condensation of vapors, heterogeneous reactions with gas phase oxidants, and photochemical reactions initiated by direct solar illumination. These transformations lead to changes in physical and optical properties, impacting the effects of aerosol in the atmosphere. Aerosol containing light-absorbing compounds will have a warming effect on the atmosphere and may undergo additional photochemical transformations.

Using a newly developed particle levitation chamber (1) coupled with optical spectroscopy and mass spectrometry methods, the physical and chemical characteristics of light absorbing aerosol samples will be explored. Initial measurements focus on classifying the absorption properties of humic acid using Mie resonance spectroscopy, a broadband scattering technique capable of resolving both size to nanometer precision and complex refractive index. A sample droplet of radius on the order of 4 μm will be prepared from a dilute solution using a microdroplet dispenser and confined in the electric fields of a linear quadrupole EDB. The sample will be illuminated with focused light from an LED and the 180° back-scattered light will be collected by a fiber optic coupled to a spectrometer (Princeton Instruments FERGIE). Over a wide range of illumination wavelengths, both the scattering and absorbing properties as a function of wavelength may be determined by comparing the spectra with predictions from Mie theory (2).

These measurements will provide crucial data describing the optical scattering of aerosol particles, and will pave the way for future measurements to explore the evolution of optical properties as samples evolve by heterogeneous or photochemical reactions. Using this experimental framework, the influence of these transformations on the physical properties of the sample will also be explored, providing a comprehensive understanding of the coupling between composition and physical and optical properties.

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3UA.1

An Enhanced Submicron Aerosol Event over Long Island and the NYC Metro Area during LISTOS 2018: Influence of a Heat Wave and Marine Air Masses. Jie Zhang, John Mak, Ziran Wei, JAMES SCHWAB, *University at Albany, SUNY*

The Long Island Sound Tropospheric Ozone Study (LISTOS) was carried out in the summer of 2018 to help researchers, regulators, and policy makers characterize and understand the circumstances leading to ozone NAAQS exceedances in the NYC Metro and Long Island area. During this campaign period in the summer of 2018, the Metro NYC and LI area suffered enhanced aerosol events in association with high ozone, with the highest daily PM₁ value (32 $\mu\text{g m}^{-3}$) approaching the daily EPA standard for PM_{2.5} (35 $\mu\text{g m}^{-3}$). The enhanced ozone and aerosol event between 06/29-07/04 was selected for study due to its long duration and its occurrence during an intense heat wave. Using our Aerodyne HR-ToF-AMS measurements from the Flax Pond Marine Laboratory near Stony Brook, Long Island, data was analyzed for the time period of 06/25-07/09, which includes the enhanced oxidant and aerosol event (06/29-07/04) and other background cases, such as plumes from the mainland, marine locations, and fireworks displays. The PMF analysis of the aerosol mass spectra identified three organic factors from the aerosol organic compounds-MOOOA, LOOOA and HOA. The LOOOA shows strong correlation between the sum of 4 kinds of gas phase VOC species (acetaldehyde, methanol, acetone, and toluene) with an R^2 of 0.63, implying these species and the LOOOA may have same source (possibly from transported urban plumes) or that these VOCs may be the precursors of the measured LOOOA. Nine sub-periods are divided out from the whole period, including four for the enhanced oxidant and aerosol event. The aerosol properties during each sub-period are analyzed, including the aerosol compound mass concentrations, mass fractions, size distributions, and organic oxidation states. The influence of the southerly winds from the marine environment is explored using measurements of the methyl sulfonic acid (MSA) mass concentration. In particular, MSA is enhanced during the heat wave influenced period and showed similar variation to the MOOOA. These results revealed detailed aerosol evolution and processing during this dramatic heat wave influenced period in the NYC area, which can also provide clues for other urban cities with similar conditions.

3UA.2

Submicron Aerosol during Autumn 2018 in the Most Polluted Megacity: The Delhi Aerosol Supersite Study (DAS). KANAN PATEL, Sahil Bhandari, Shahzad Gani, Purushottam Kumar, Gazala Habib, Joshua Apte, Lea Hildebrandt Ruiz, *University of Texas at Austin*

New Delhi, India is the most polluted megacity in the world and routinely experiences high aerosol concentrations. In particular, the autumn season (mid Sep-Nov) experiences some of the highest concentrations which has been hypothesized to be due to agricultural burning of the “kharif” crops in the Indo-Gangetic plains, and transitional meteorology (between monsoon and winter) during this period. As part of the Delhi Aerosol Supersite Study, NR-PM₁ concentrations and composition have been measured using an Aerosol Chemical Speciation Monitor (ACSM) from January-2017 to present which includes autumn 2018.

In autumn 2018, the average NR-PM₁ concentration increased from ~55 µg/m³ in the last two weeks of September to ~210 µg/m³ in November-2018. On November 5 (around the time of the festival of Diwali), the NR-PM₁ concentration reached ~1100 µg/m³, highest in the 26 months of data collection. On average, organic aerosol (OA) constituted 68.7% while the inorganics, sulfate, nitrate, ammonium and chloride constituted 12.4%, 8.6%, 8.7% and 1.6% of NR-PM₁ respectively during this season.

We performed source apportionment by using Positive Matrix Factorization on the OA data measured by the ACSM. Three factors—HOA (Hydrocarbon-like-OA), BBOA (Biomass-Burning-OA) and OOA (Oxidized-OA) were resolved. While BBOA dominated during episodic events, on average, all the factors contributed comparably (OOA—37%, BBOA—33% and HOA—30%), indicating equal importance of traffic (HOA), biomass-burning (BBOA) and secondary OA (OOA) during this season. Additionally, ~70% of 95th percentile BBOA concentration events during this season were associated with N and N-W wind directions, pointing towards the role of agricultural burning from the N-W states of Punjab and Haryana. Thus, our analysis provides insights into sources that influence submicron aerosol concentrations during an extremely polluted season in Delhi.

3UA.3

Spatial and Seasonal Trends in Polycyclic Aromatic Hydrocarbon Particulate Measurements in Ulaanbaatar, Mongolia. Skyler Simon, AUDREY DANG, Jay R. Turner, Rufus Edwards, Brent Williams, *Washington University in St. Louis*

Ulaanbaatar, Mongolia is globally the coldest capital city. Poor wintertime air quality is influenced by distributed space heating (including inefficient residential coal stoves) and other emission sources, strong inversions, and a topography that further traps ground-level emissions. Ambient PM_{2.5} field sampling was conducted January to April 2013 across four sites with offline analysis for chemical components. More recently, a subset of 80 archived samples (20 samples per site) were analyzed by Filter Thermal desorption Aerosol Gas Chromatography – Mass Spectrometry (Filter TAG) for organic species including particle-bound polycyclic aromatic hydrocarbons (PAHs). To date 18 PAHs have been quantified using authentic standards and surrogate standards, and additional unquantified PAH material is present in the samples. The grand average (across all sites and sampling dates) 24-hour integrated summed ΣPAHs was 1.3 µg/m³ (range 0.1-4.6 µg/m³) with strong seasonal variation in both concentration and carcinogenic potency. ΣPAHs spatiotemporal variability across the four sites was characterized by Pearson correlation coefficients 0.84-0.92 and coefficients of deviation (COD) 0.18-0.35; these metrics demonstrate relatively high homogeneity across the city. Positive matrix factorization (PMF) was used to resolve PAH sources and atmospheric processes.

3UA.4

Possible Heterogeneous Chemistry of Hydroxymethanesulfonate (HMS) in Northern China Winter Haze. SHAOJIE SONG, *Harvard University*

Chemical mechanisms responsible for rapid sulfate production, an important driver of winter haze formation in northern China, remain unclear. Here, we propose a potentially important heterogeneous hydroxymethanesulfonate (HMS) chemical mechanism. Through analyzing field measurements with aerosol mass spectrometry, we show evidence for a possible significant existence in haze aerosols of organosulfur primarily as HMS, misidentified as sulfate in previous observations. We estimate that HMS can account for up to about one-third of the sulfate concentrations unexplained by current air quality models. Heterogeneous production of HMS by SO₂ and formaldehyde is favored under northern China winter haze conditions due to high aerosol water content, moderately acidic pH values, high gaseous precursor levels, and low temperature. These analyses identify an unappreciated importance of formaldehyde in secondary aerosol formation and calls for more research on sources and on the chemistry of formaldehyde in northern China winter. This paper has recently been published in *Atmospheric Chemistry and Physics*.

3UA.5

Assessment of Airborne Toxic Metals at an Environmental Justice Community in Wilmington, Delaware. Olivia Ryder, Jennifer DeWinter, STEVEN G. BROWN, Elizabeth Frey, Keith Hoffman, *Sonoma Technology, Inc*

It is well established that prolonged exposure to particulate matter (PM) containing toxic metal species can have negative health implications. In this study, we attempt to identify the sources of toxic metals in aerosols sampled at the environmental justice (EJ) community of Eden Park, DE. The community is in the 88th percentile nationally for EJ index of cancer risk, and the 90th percentile for EJ index of PM_{2.5} exposure. It is surrounded by many potential sources of metal pollution including industrial facilities, the Port of Wilmington, and a highly trafficked freeway. We used hourly measurements of multiple metals using an Xact 625i plus measurements of meteorology, black carbon, PM₁₀, PM_{2.5}, NO_x, and SO₂ to determine the ambient concentration of toxic air pollutants and to apportion their sources. Conditional bivariate probability function maps and time variance maps were constructed using the OpenAir package and EPA Positive Matrix Factorization was used to determine the sources of the measured metals. We found that average concentrations of toxics such as arsenic and lead were comparable to nearby routine measurements, but that transient concentration events occurred intermittently where As and Pb concentrations were more than an order of magnitude larger than the study average. With PMF, we found 3 sources: soil/dust, concrete manufacturing, and vehicles emissions. Overall the local industry and intermodal traffic emissions are large contributors to the ambient air pollution in the community, though transient, high concentration events from other sources are also surprising and important.

3UA.6**Characterization of Particulate Matter in Summer Using High-Resolution Aerosol Mass Spectrometry in San Antonio.**

FANGZHOU GUO, Alexander Bui, Edward Fortner, Benjamin Schulze, Sujan Shrestha, Subin Yoon, Rebecca J. Sheesley, Sascha Usenko, Tara Yacovitch, James Flynn, 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 cities in the country over the past decade. As demonstrated by an ozone design value in violation of the federal threshold, 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 deployed a mobile air quality laboratory (MAQL) in locations to the southeast (Traveler's World RV Park (TW)) and northwest (University of Texas at San Antonio campus (UTSA)) of downtown San Antonio in May, 2017. Aerodyne's mobile laboratory (AML) was also deployed at UTSA and measuring during May 12 – 16 and 27 – 31. Chemical characterization of non-refractory submicron PM (NR-PM₁) was conducted using two Aerodyne high-resolution time-of-flight aerosol mass spectrometers (HR-ToF-AMS) at each site. 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. Results from both HR-ToF-AMS indicate large organic and sulfate aerosol plumes, with maximum 1-minute averaged concentrations of 35.65 and 11.30 µg/m³ respectively. At TW site, PMF analysis of the high-resolution spectra identifies hydrocarbon-like OA (HOA, 14.2%), a less oxygenated OA (LO-OOA, 48.4%), and a more oxygenated OA (MO-OOA, 37.4%), which allows us to estimate the fraction of PM in San Antonio in summer that is local and anthropogenic. A Lagrangian analysis is being performed to quantify the variations in chemical composition, aging processes of organic aerosol, and potential source factors of organic portion of NR-PM₁ across the city.

4JS.1

Sahil Bhandari, Ph.D. Candidate in ChemE (UT Austin), Looking for Post-Doc Positions (Agency/National Labs/Industry), Prefer California and Massachusetts. SAHIL BHANDARI, *University of Texas at Austin*

Over the past three years of field measurements, air quality modeling and high time resolution data mining in the software Igor, I have been working as a part of a collaborative research effort, led by professors in civil and chemical engineering, called the Delhi Aerosol Supersite campaign. My work focuses on the apportionment of air pollution to multiple factors such as climatology, photochemical formation, sources local to and upwind of the city as well as contributions of long-range transport. Additionally, I am working on the quantification of modeling errors in Positive Matrix Factorization due to its inability to capture non-linearity effects. Parallely, I have modeled chamber experiments using the Carbon Bond Mechanism (CB6r2) in the atmospheric chemistry framework SAPRC for our research group, leading to two second-author publications. Moreover, I am familiarized with instrument development (TD-CAPS), remote sensing and geospatial modeling tools (ArcGIS, ERDAS Imagine) as well. Together, my work on the identification of particulate matter sources in Delhi, quantifying personal exposure in different microenvironments in Austin, and estimation of emissions of greenhouse gases in West Texas has the potential to impact 50 million people. In total, I expect at least three first-author and five second-author publications from my research.

Anticipated Availability: Beginning Fall 2020

Geographic Preference: California and Massachusetts

I believe that a keen interest in environmental research, consulting, and management, the ability to work in challenging research environments, a diverse skill set, and experience with both academic research and consulting projects make me a candidate worthy of consideration. I am particularly fascinated by the fat tail phenomena in emission inventories, the glaring gaps in top-down and bottom-up emission estimates for primary pollutants, and the potential of low-cost sensors and remote sensing in environmental monitoring and policy development.

4JS.2

Meet the job seeker: Shahzad Gani. SHAHZAD GANI, *University of Texas at Austin*

Bio: Shahzad Gani has a BTech in Civil Engineering from the Indian Institute of Technology Delhi and an MS in Environmental Engineering from the University of Texas at Austin. He is currently a doctoral candidate at the University of Texas at Austin where he seeks to understand the sources and processes that drive urban air pollution.

Key interests: (i) Atmospheric Science (ii) Air pollution exposure, (iii) Atmospheric aerosol dynamics, (iv) Science communication.

Key skills: (i) Designing and executing long-term air pollution measurement field campaigns, (ii) Setting up and operating range of air quality instrumentation—low-cost to state-of-the-art, (iii) Complementing field measurements with satellite and modeling datasets, (iv) Processing, analyzing and visualizing large datasets.

Job interest: Postdoc

Geographical preference: Boston, Massachusetts

Preferred start date: January 2020

Contact: shahzadgani@utexas.edu

Note: Not a US citizen or permanent resident.

4JS.3

Kaisen Lin, PhD Student at Virginia Tech Looking for Post-doc Positions. KAISEN LIN, *Virginia Tech*

My name is Kaisen Lin. Under the direction of Dr. Linsey Marr, I am completing my Ph.D. in Environmental Engineering at Virginia Tech with an expected degree date of May 2020. I am interested in post-doctoral positions.

My dissertation investigates the effects of relative humidity on the viability of airborne microorganisms. Understanding the viability of infectious agents at various environmental conditions is essential for control of infectious diseases transmission. In this interdisciplinary work, I looked into the relationship between relative humidity and the viability of airborne bacteria and viruses. To explain the observed patterns, I investigated the evaporation rate of droplets and the resulting changes in their solute concentrations over time at various relative humidity levels. I am currently manipulating the chemical composition of droplets and figuring out the main variable that affects the viability of airborne microorganisms. I have learned a variety of skills from this project, including operating particle sizing instruments, e.g. SMPS and APS, utilizing different bioaerosol samplers, conducting biological assays for microbe quantification, visualizing droplets and microbes using microscopy, and understanding particle evaporation/condensation processes.

My future research interests lie at the intersection of airborne microorganisms and chemistry and composition of atmospheric aerosols. I am particularly interested in studying how the chemical characteristics of atmospheric aerosols affect the viability of airborne microorganisms, and the role of atmospheric chemistry in shaping microbial community.

4JS.4

Raj M. Lal, Graduate Student Georgia Tech/PhD, Post-Doc/Air Quality, Sustainability. RAJ LAL, *Georgia Institute of Technology*

- a) Job Type of Interest: (Post-Doc) Air Quality, Sustainability, Environmental Policy
- b) Anticipated availability: Spring 2020. Graduation planned for Fall 2019
- c) Geographic Preference: None

My previous work includes characterizing how emissions from biomass burning is discoloring the Taj Mahal, an iconic Indian monument and one of the Seven Wonders of the World. Here, I generated on-site, spatially-resolved emission inventories for municipal solid waste (MSW) and dung cake burning, and used AERMOD to simulated PM_{2.5} impacts in Agra and found that MSW burning was the leading contributor to pollutant deposition of the biomass sources (Lal, 2016, Environmental Research Letters). I have also been part of a team that assessed the potential of urban-industrial symbiosis strategies for carbon mitigation with local health co-benefits in China. In this work, I modeled air pollution impacts of novel, waste heat re-use strategies for each province in China. We found that these policy strategies can reduce PM_{2.5}-induced premature mortality between <1% and 47% in Chinese cities (Ramaswami, 2017, Nature Climate Change). Historically, mobile sources have been a leading contributor to ambient pollution in US cities, leading to elevated levels of pollution near major roadways. I compared regulatory monitors in the US from the EPA Near-road (monitoring) Network to other monitors in US cities and found there is no statistical difference ($\alpha=0.05$) between PM_{2.5} near-road and the elsewhere in cities (Lal, 2019, in review). My current work includes exploring the link between air quality (as measured with low-cost sensors and simulated in R-Line, the EPA mobile source dispersion model), neighborhood infrastructure, and subjective well-being in a US city (in prep). In addition, I'm using Geos-Chem to simulate air quality in India.

4JS.5

Nirmala Thomas, Ph.D. Candidate, Postdoc. NIRMALA THOMAS, *Rutgers University, New Brunswick, New Jersey*

Research Interest: We are well aware of adverse health effects caused by ambient air pollutants; those negative effects are further amplified by our exposures to indoor pollutants, especially since we spend about 90% of our time indoors. My research interest is to connect our investigation of aerosol and bioaerosol exposures in indoor and outdoor environments with health symptoms and properties of the environments, e.g., environmental variables and/or design, structural anomalies, and maintenance practices of the built environments. Given that multiple factors affect our exposures to aerosols and bioaerosols, there is a need to improve our ability to measure such exposures in both indoor and outdoor environments using advanced stationary and personal samplers and then integrate the exposure data with building characteristics, environmental parameters, and people's health.

Thesis work: I already investigated the potential to use, integrate, and correlate three different data streams (i.e., traditional indoor air quality investigation, use of questionnaires and spatially resolved infrared thermography imaging) during indoor air quality investigations in residential multi-apartment buildings and then use the integrated data to investigate the effect of building deficiencies on indoor air quality and residents' health. I also examined factors affecting the presence and spatiotemporal variability of airborne bacteria and fungi in three multi-apartment residential buildings with different heating and ventilation system types. In an ongoing work, I am examining the ability of existing and new personal samplers to determine personal bioaerosol exposures in indoor and outdoor environments accurately. The samplers are used in distinctly different locations, and the collected samples are examined using epifluorescence microscopy, hemocytometer cell counting, flow cytometry, and culturability assay.

Anticipated Availability: Summer/Fall 2020

Job types of interest: Post-doc, Government

Geographical preferences: None

4JS.6

Dana McGuffin, Current PhD Candidate seeking Postdoc in Atmospheric Inverse Modelling. DANA MCGUFFIN, *Carnegie Mellon University*

I am a 4th-year Ph.D. student in the Department of Chemical Engineering at Carnegie Mellon University, working with Professors Peter Adams and B. Erik Ydstie. I am motivated to answer questions about atmospheric science by utilizing data assimilation techniques that combine models with measurements.

Uncertainty in predicted concentration of atmospheric aerosol is a major source of the uncertainty in climate change estimates. Chemical transport models (CTMs) predict the global concentration field of atmospheric aerosol mass and number. However, CTM predictions are often biased relative to field measurements due to uncertainty in CTM processes and model inputs, such as particle formation and aerosol emission inventories, respectively. In general, field measurements can be systematically integrated with a CTM to estimate the uncertain model input (i.e. emission inventory) using inverse modeling techniques, such as the Kalman Filter and adjoint method. These conventional inverse methods are not ideal for integrating field measurements of the particle number size distribution because of complexities in the general dynamic equation and large computational effort required to capture those complexities.

The aim of my thesis is to utilize techniques from the area of process control to estimate uncertain aerosol dynamics using measurements of the particle number size distribution. In the field of process control, an observer "observes" or estimates previously unknown or uncertain variables in a system based on feedback from measurements. Commonly, this method can be found calibrating controllers in chemical plants, but I use it to calibrate atmospheric models.

I am seeking a research position in the field of atmospheric inverse modeling to develop new algorithms or apply inverse modeling methods that improve model predictions by incorporating measurements. My career plan involves developing and applying cutting-edge data assimilation techniques to atmospheric models as a research scientist in a national lab's atmospheric or Earth Science division.

4JS.8

Job Seeker Abstract for Jessica Mirrielees. JESSICA MIRRIELEES, *Texas A&M University*

My name is Jessica Mirrielees. I have a B.S. in Chemistry from the University of Texas at Austin and a M.S. in Atmospheric Science from Texas A&M University, and I am currently working on my Ph.D. in Atmospheric Science, also at Texas A&M University.

My research interests include aerosols (including marine aerosols), cloud condensation nuclei, and instrumentation. I have taken part in field campaigns and lab studies; these projects include the North Atlantic Aerosols and Marine Ecosystems Study with NASA, mesocosm studies that employ a Marine Aerosol Reference Tank to study the effect of phytoplankton blooms on aerosol concentration and properties, and a project on ice nucleation instruments with the Fifth International Workshop on Ice Nucleation. I also have experience with data analysis, MATLAB, instrument repair, and Raman spectroscopy.

My anticipated graduation date is in August 2020. I am looking for a position that I can start in September 2020, specifically a post doc position in aerosol, atmospheric chemistry, or cloud microphysics research in a laboratory setting. I am interested in positions that will allow me to gain more experience with aerosol instruments and data analysis, in either government or industry. I would prefer to work in the United States, and I am open to relocating.

4JS.9

Anna Hodshire, PhD candidate, Postdoctoral Position. ANNA HODSHIRE, *Colorado State University*

My research to date has been focused on modeling aerosol microphysics, nucleation, early stages of particle growth, and gas-phase oxidation chemistry. I have applied these skills to variable environments, including in smoke plumes, the Southern Great Plains of the U.S., within the Amazon and a ponderosa pine forest, in the upper tropical troposphere, and over the remote oceans. I anticipate graduating next spring from Colorado State University with a PhD in Atmospheric Science and will be available starting the summer of 2020. To date, I have worked with a number of box models that focus on aerosol microphysics and/or gas-phase chemistry as well as the GEOS-Chem global/regional chemical transport model coupled to a microphysical module (TOMAS). I currently am seeking a postdoctoral position either in an academic setting or government lab but am also open to consulting positions. My main goal as a postdoc or similar position is to learn new sets of tools and areas of expertise, complimenting my existing skill set. New skills that I'm interested in include, but are not limited to, new types of models or modeling techniques (such as inverse modeling, machine learning) and new regions of the globe (such as the stratosphere, urban environments, high latitude free troposphere).

4JS.10

Jenna Ditto, PhD Student, Postdoctoral Fellowship. JENNA DITTO, *Yale University*

The focus of my doctoral research has been on characterizing the evolution of complex functionalized mixtures of organic compounds. I am interested in leveraging high resolution mass spectrometry to accomplish this at the molecular level; using offline sampling and a combination of gas and liquid chromatography with high resolution mass spectrometry, I am currently investigating key elemental and structural features of aged organic compounds in the atmosphere. A particular emphasis of my current research is the characterization of functionalized organic compounds from mixed biogenic and anthropogenic sources (including nitrogen- and sulfur-containing species) across the volatility spectrum—something that I hope to pursue after graduate school as well. Moving beyond my PhD, I aim to continue to probe the evolution of multiphase organic mixtures at the molecular level, but seek to broaden my skills and gain experience with a wider range of online mass spectrometry techniques. Ultimately, I am interested in learning more about how to distill and synergize the strengths of high chemical resolution measurements with high time resolution measurements for improved atmospheric chemistry modeling. I seek a postdoctoral fellowship—I anticipate graduating in the summer of 2020, and will be available to begin a new position in late summer or early fall of 2020.

4JS.11

I'm Looking for a Post Doc Position. GREGOR KOTALCZYK, *University Duisburg-Essen*

My area of expertise is the modelling and numerical simulation of particulate processes encountered in industrial applications – although similar techniques could be used to describe the complex mechanisms observed in atmospheric systems (as we have shown in a recent publication).

At the moment, I'm finishing my PhD thesis (in chemical engineering) and am employed at the University of Duisburg-Essen in the group of Prof. Einar Kruis (the successor of Prof. Heinz Fissan). During my PhD thesis I focused primarily on the GPU- based Monte Carlo simulations for the solution of population balances within compartmental models. However, different other simulation techniques as the sectional methods, as well as the fixed- pivot simulation techniques have been at the focus of my interest as well.

Prior studies in physics (I have obtained a diploma in physics in the year 2013 at the Humboldt University of Berlin), have given me the opportunity to gather a deep knowledge on stability analysis of dynamical systems and stochastic processes. This skill set has helped me to design new Monte Carlo methods and GPU-algorithms for the simulation of particulate processes.

I would like to extend my areas of expertise by learning novel simulation techniques (such as CFD, DEM, etc.), I would also be interested on the tuning of the underlying simulation algorithms of these techniques at the most basic level – as well as on the combination of those with a compartmental population balance model.

I am also interested in programming larger computational architectures as well as high performance computing in combination with novel computational languages such as Julia.

4JS.12

Zezen, Ph.D. of Engineering, Postdoc or Research Scientist Position. ZEZHEN CHENG, *University of Georgia*

I have achieved my B.S. of Chemical Engineering degree from the Ohio State University and Master of Chemical Engineering degree from Carnegie Mellon University. Now I am pursuing my Ph.D. of Engineering degree at the University of Georgia. My Ph.D. research focus on the light-absorption properties of fresh and aged combustion carbonaceous aerosols including black carbon (BC) and brown carbon (BrC).

I contributed to designing, building, and testing a controlled combustion system, where we can generate combustion carbonaceous aerosols with variable light-absorption properties via changing combustion conditions (e.g., air to fuel ratio and combustion temperature). This system has an advantage that it can generate emissions with a narrower distribution of chemical, physical, and optical properties than the emissions in real-life combustion. We then used the system to perform controlled combustion experiments with toluene and benzene as model fuels. These experiments showed that the light-absorption properties of the emissions are strongly correlated with combustion conditions, and the emitted aerosols exhibit a continuum of light-absorption properties regardless of fuel type.

Currently, I am working on investigating the evolution of light-absorbing Polycyclic Aromatic Hydrocarbons (PAHs) due to oxidation by NO₃, as part of a collaborative project with Aerodyne Research Inc. We generated light-absorbing PAHs with variable light-absorption properties from toluene combustion at different combustion conditions. We then exposed the PAHs to different concentrations of NO₃ in an oxidation flow reactor and investigated the evolution of their chemical, physical, and optical properties. We are currently in the data analysis phase of the project.

I expect to graduate in May 2020. I am seeking a postdoc or research scientist position in the field of primary and secondary aerosol characterization. I do not have any geographical preferences.

4JS.13

Yunle Chen, Ph.D. Student Seeking Postdoc Positions in Academia or Industry. YUNLE CHEN, *Georgia Institute of Technology*

I am a Ph.D. student from Georgia Tech with aerosol chemistry background. I have worked on both field and laboratory studies in the past four years. I am experienced in aerosol characterization, environmental chamber studies, and data analysis for online mass spectrometry instruments.

My research projects include:

- 1) Method development: response of HR-ToF-AMS to inorganic sulfate and organosulfur compounds, where I developed a method to estimate the abundance of organosulfur based on HR-ToF-AMS measurements;
- 2) Field study: OA composition at a rural site in southeastern U.S., where I focused on obtaining new insights into SOA evolution by combining HR-ToF-AMS and FIGAERO-HR-ToF-CIMS measurements, with the use of OA factorization analysis;
- 3) Chamber SOA study: small organic acid formation from BVOC oxidation, where I aim to investigate small organic acid formation mechanism and explain the gap between model predictions and ambient measurements of organic acids;
- 4) Aerosol health effects (secondary role): health effects of laboratory-generated SOA from different precursors, where we evaluated the health effects of SOA generated from different VOC systems using both chemical and cellular assays.

My anticipated graduation is around spring 2020. I am interested in post-doc level positions in academia or industry. I do not have any geographical preference. I am comfortable to continue as an experimentalist but am also willing to take up new challenges.

4JS.14

Fangzhou Guo, PhD Candidate at Rice University (Current), Looking for Postdoc Position in Aerosol Chemistry (AMS Related). FANGZHOU GUO, *Rice University*

I am currently a 4th year PhD candidate in Dr. Rob Griffin's group at Rice University. My research focused on the sources and formation of O₃ and non-refractory submicron particles (NR-PM₁) in San Antonio and the temporal differences of the two criteria pollutants under varying meteorological conditions.

Funded by the Texas Commission on Environmental Quality, my collaborators and I deployed the Mobile Air Quality Laboratory to San Antonio for four weeks during May 2017, measuring O₃, NO_x, NO_y, CO, SO₂, NR-PM₁ (with HR-ToF-AMS), VOCs (with PTR-MS and canisters), and meteorological parameters. I utilized the TUV Model and NASA Langley Research Center (LaRC) 0-D Box Model to quantify the diurnal variations in O₃ production rate, efficiency (OPE), OH reactivity of VOCs, and O₃ production regime across the city. Analysis of NR-PM₁ data is performed using SQUIRREL and PIKA in Igor Pro, followed by Positive Matrix Factorization (PMF) for source apportionment on the high-resolution mass spectral, whereas aerosol liquid water content and pH are modeled using ISORROPIA-II. Cluster analysis and Weighted Potential Source Contribution Function (WPSCF) analysis are done with HYSPLIT to identify the regional sources of gaseous and particle pollutants. Furthermore, the relationship between local O₃ production and SOA formation is evaluated and a Lagrangian analysis is developed to quantify the variations in composition and oxidation processes of organic aerosol across the city.

My anticipated graduation is May 2020. I am looking for a Postdoc researcher position in aerosol chemistry, especially field and lab studies emphasized on SOA formation and source apportionment using AMS or similar instruments. I am also interested in instrument development and the nexus between criteria air pollutants (e.g. PM and O₃) and human health. I have no geographical preferences and am willing to travel for field campaigns.

4JS.15

Nisar Ali Baig, Research Associate, MS Thesis. NISAR ALI BAIG, *IIT-DELHI*

I have been working in research for almost 3 years in IIT Delhi under Dr. Gazala Habib, Civil Department. I have done field sampling and setting up the temporary lab at field site. I know how to handle things when you are on field work. My experience includes handling of Air instruments that gives Number and Mass concentration, Size distribution, Black carbon concentration and Chemical speciation. I have experience of health instrument also as I was involved in two projects that comes in "Aerosol and health". Chemical analysis is another part of the experience. Also, I kept myself involved in data analysis. My work has been presented in three international conferences, namely AAAS (American Association for Advancement of Science), EAC (European Aerosol Conference) and IAC (International Aerosol Conference).

Currently, I am working as "Research Associate" in IIT Delhi under Dr. SAGNIK DEY, Centre for Atmospheric Science. After having experience of all these years and working on many instruments, I realized that proper knowledge of instruments is very important in any research. So, my current interest is instrumentation. I want to learn more about instruments so that I can deal with any problem that comes in field work and also to make it sure that the data I am getting is most reasonable.

I am looking forward for MS thesis in instrumentation or as Research Associate in the project. I really love to join a group that love to share knowledge and experience and to make networking to explore other research around the world.

4JS.16

AAAR job seeking: Zechen Yu is Looking for PostDoc Position in Air Quality Modeling. ZECHEN YU, *University of Florida*

I am currently a Ph.D. candidate at University of Florida and I will graduate in Summer 2019. My Ph.D. research is developing a box model to characterize and simulate multiphase reactions of inorganic and organic compounds in atmosphere, especially in the presence of airborne dust particles. I am also familiar with the operation of large outdoor smog chamber, collecting data from on-line and off-line instruments to measure PM, and analyzing the chamber data. The chemistry box model that I developed was coded in Fortran computer language. I am currently working on the integration of chemistry box model into regional air quality models, such as CAMx.

For my future research interest, I aim to study the multiphase chemistry of secondary inorganic and organic aerosols and using box model and regional models to explore their impacts on air qualities and human health.

I am seeking for a postdoctoral position starting in fall of 2019 or early spring of 2020 and no special geographical preferences.

Email: yuzechen@ufl.edu

Personal Website: <http://zechen.ddns.me>

4JS.17

Julia Bakker-Arkema, Ph.D. Candidate in Analytical, Environmental, and Atmospheric Chemistry, Seeking Government or Academic Postdoctoral Position. JULIA BAKKER-ARKEMA, *University of Colorado*

I am currently a graduate student in the Ziemann Group at the University of Colorado. My Ph.D. research has focused on the mechanisms of volatile organic compound (VOC) oxidation to form secondary organic aerosol (SOA), and the kinetics of heterogeneous and multiphase aerosol chemistry processes. I have primarily conducted laboratory research centered on environmental chamber studies of VOC oxidation, and I've gained experience with an array of analytical methods to study the gas- and particle-phase products including multiple chromatography and mass spectrometry techniques. As an analytical atmospheric chemist, I'm interested in taking advantage of a broad range of instrumentation to develop a more complete understanding of the chemistry of the atmosphere. I plan to graduate in December of 2019, and I'm seeking a postdoctoral position.

4JS.19**Tianren Wu, Ph.D. Student, Seeking Postdoctoral Position.**TIANREN WU, *Purdue University*

I am a Ph.D. candidate in Civil Engineering at Purdue University conducting research on indoor and urban aerosols and indoor air quality. I will complete my Ph.D. studies in May 2020. I enjoy research on aerosol characterization using state-of-art techniques. I would like to continue novel research on aerosol science as a post-doctoral scholar in academia or at a national laboratory.

My doctoral research is aimed at characterizing aerosol and VOC dynamics in buildings and their HVAC systems. The first phase of my research is focused on measurement of bioaerosols using online laser-induced fluorescence (LIF) techniques. I evaluated infant crawling-induced resuspension of bioaerosol using a mechanical crawling infant and characterized the impact of occupants on bioaerosol emissions and size distributions in a realistic office environment. Next, I investigated indoor new particle formation (NPF) and measured the size distributions of sub-3 nm aerosol in an occupied office under different building ventilation modes. Real-time measurements of VOCs were also conducted using PTR-TOF-MS to probe human- and non-human-related emissions and the interactions of VOCs with aerosols and surfaces. As the HVAC system plays an important role in shaping indoor chemistry, a multi-location VOC sampling system was developed to characterize VOC deposition onto HVAC filters and duct surfaces. The third part of my research is on the evaluation of the in-situ performance of HVAC filters in their removal of aerosols from 1.5 nm to 20 μm in a full-scale building ventilation duct. The morphological features and phase state (bounce factors) of the aerosols are monitored online to understand their impact on filtration performance.

I am familiar with the measurement and analysis of VOCs using an IONICON PTR-TOF-MS, measurement of sub-3 nm aerosol with a Half-mini DMA and Airmodus nCNC, characterization of aerosol morphological features and charging state using DMA-CPMA and DMA-ELPI+ setups, and investigating aerosol phase state via bounce factors measured by an ELPI+. I have a great passion for lab experiments. In the future, I would like to learn advanced skills and conduct lab and field experiments to probe aerosol formation and their interaction with gas-phase species.

4JS.20**Seeking a Faculty Position in Environmental Science and Engineering.** YUANLONG HUANG, *California Institute of Technology*

The field of atmospheric aerosol chemistry and physics is undergoing rapid growth. Owing to emerging novel experimental techniques, new mechanisms of particle formation and evolution are being revealed. Nonetheless, understanding of the transformation from vapor molecules to airborne particulate matter remains incomplete. New techniques, including computational simulation and advanced instrumentation, will continue to revolutionize the field of atmospheric chemistry. My Ph.D. studies in the Caltech atmospheric chemistry laboratory have involved design and characterization of atmospheric reactors, development of mathematical models of gas and aerosol behavior, and conception and construction of new instruments, each of which are crucial to a fundamental understanding of atmospheric aerosol formation. I am now a postdoctoral fellow in the Seinfeld lab at Caltech working on projects on aerosol capture/detection techniques and vapor-particle interaction mechanisms. I am also conducting atmospheric chemical transport model simulations by incorporating the latest parameters derived from laboratory studies to evaluate our understanding of aerosol formation. At the same time that I have been doing research, I have also enjoyed mentoring students (the Caltech summer undergraduate research fellows and the younger graduate students in the group) in the laboratory and in the classroom (teaching assistant for the aerosol physics and chemistry courses). I am seeking a faculty position in the field of environmental science and engineering. I have had a great experience in teaching through serving as a Graduate Teaching Assistant. In research, I will carry out novel experiments in atmospheric chemistry and aerosol formation, share my research experience with the next generations, and, most importantly, call for attention to improving air quality by providing new knowledge to both the public and policymakers.

4JS.21

Meet the Job Seekers: Danielle C. Draper. DANIELLE C. DRAPER, *University of California, Irvine*

The majority of my research to date has focused on understanding the nuances of secondary organic aerosol formation (SOA) from NO₃ radical oxidation of monoterpenes – an atmospheric process that occurs at the confluence of biogenic and anthropogenic emissions. Projects have ranged from ambient observations of organic nitrates in the gas- and particle-phase, to chamber studies of NO₃ + various monoterpenes to characterize SOA yields, to developing a detailed chemical mechanism leading to potentially condensable species from Δ-carene + NO₃ using computational chemistry. I consider myself to be a question-oriented scientist, having found enormous value and enjoyment in pursuing a relatively narrow scientific question using a broad range of tools and approaches. My methodologically broad experience has been a valuable way to pursue scientific questions, and has led to increased confidence in pursuing techniques outside of my current expertise. As a current graduate student, I am seeking a postdoctoral position with expected availability starting summer 2020 and am flexible geographically. During my postdoc, I hope to take on a new (to me) question within the field of atmospheric chemistry and to continue developing proficiency with new tools to further broaden my resources for future research. I am ultimately hoping for a faculty position at either a research institution or a primarily undergraduate institution with a strong focus on research.

4JS.22

Jai Prakash; Visiting Research Scientist, PhD, Faculty Position/Research Scientist. JAI PRAKASH, *Washington University in St. Louis*

I am an environmental engineering graduate with expertise in atmospheric aerosol and its physical and chemical properties. In total, I have research experience of 8+ years in atmospheric aerosol, microphysical, chemical and optical characterization. In my Ph.D. work, I developed portable dilution sampler (PDS) to achieve complete gas-to-particle partitioning at a given residence time and dilution ratio. This is a very valuable technology for multi-pollutant emission measurements from mobile and stationary sources. I also developed new PM_{2.5}, OC, and EC emission factors of on-road transport sector in the Indian context and estimated spatial emission inventory for fine aerosol and its precursors involving new Tier-III approach. Currently, I am visiting Research scientist at Washington University in St. Louis. My current research and expertise in advance receptor modeling tool for real-time data analysis and source apportionment using Positive Matrix Factorization (PMF), Condition probability Function (CPF) and Potential Source Contribution Function (PSCF). I have an acquaintance of real-time instrument handling on Xact-625i real-time ambient trace metal monitor, Time-of-Flight Aerosol Mass Spectrometer (TOF-AMS), real-time total carbon analyzer (TCA-08), real-time BC-aethalometer, and low-cost sensor.

In total, I have published 10 research (+ several in the pipeline –) papers in some of the most reputed international journals of atmospheric and aerosol sciences and actively participated in 13 international aerosol conferences. Overall my research experience will give me the opportunity to develop myself as a promising candidate with high potential and internationally leading young scientist, bridging India and the United States. My primary motivation to apply job-seeker to finding faculty position and also research scientist position in the direction of aerosol chemistry, Source apportionment, Air-borne Perfluorocarbons (PFCs) and their exposure and risk apportionment.

4JS.23

Matthew Brege, PhD Candidate, Postdoc and Faculty, United States. MATTHEW BREGE, *Michigan Technological University*

I am a Chemistry PhD candidate at Michigan Tech expecting to graduate in December 2019. Trained as an analytical chemist, I have studied the detailed molecular composition of organic aerosol using ultrahigh resolution mass spectrometry and liquid chromatography-mass spectrometry. I have experience with computer software tools for assigning molecular formulas to ultrahigh resolution mass spectrometry data and I am proficient in script writing for the analysis of large data sets using R. I also have proposal writing experience and was awarded a NASA Earth and Space Sciences Fellowship.

I have studied biomass combustion influenced fog and organic aerosol to understand aqueous phase transformations of the complex mixtures. We determined the trends between different samples influenced by fresh emissions, aerosol liquid water, and fog formation. We observed an increased level of oxidation and chemical functionalization, as well as a carbon backbone degradation, with aqueous phase processing. Currently, I am studying biomass burning tar balls using multiple different mass spectrometry ionization methods to obtain the most comprehensive detailed molecular characterization possible. This work has revealed a continuum of carbonaceous species, which are comprehensive in the observed ranges of oxidation and hydrogen saturation. The observed species span nearly the entire theoretical space of possible molecular formulas for the molecular weight ranges analyzed.

In addition to research, I have been a teaching assistant for both lower and higher division Chemistry laboratory courses, including instrumental analysis, quantitative analysis and general chemistry I & II. I am interested in postdoc positions as well as faculty positions, in the United States, as well as other areas of North America and Europe.

4JS.25

Yue Zhang, NSF/NIH Postdoc at the University of North Carolina, Chapel Hill/Ph.D., Looking for a Faculty or Scientist Position. YUE ZHANG, *Univ. of North Carolina, Chapel Hill/Aerodyne Research, Inc.*

Characterizing the chemical evolution and physical properties of gases and aerosols in the atmosphere to examine their climate and health effects has been the focus of my research studies. Some of my work was to develop a new technique that could measure the in-situ physicochemical properties of aerosols, which inspired a variety of studies by different research groups. My strong interest in environmental chemistry, including the chemical properties of aerosols and the formation of organic aerosols led to my NSF sponsored postdoctoral research at UNC Chapel Hill. This work has evolved into multiple projects at a variety of institutions including MIT and UC Berkeley. My research has ranged from physical and analytical chemistry to instrument development, as well as from fundamental atmospheric chemistry to aerosol climate effects (cloud condensation nuclei and ice nucleation properties). I am also working on a research project with FDA/NIH to study the chemical composition and toxicological effects of e-cigarette aerosols, which I can apply to study environmental health in the future. My experience in field campaigns in the Amazon rainforest and Montana the FIREX project also gives me the ability to combine laboratory work with field measurement.

Besides conducting research, I very much enjoy teaching and have experience in both undergraduate and graduate level classes and laboratory sessions with students of various backgrounds. Therefore, I am looking for a faculty position in environmental sciences or chemistry at a higher education institution in the U.S. next year. To date, my research received multiple recognitions including participation in the Atmospheric Chemistry Colloquium for Emerging Senior Scientists (ACCESS), the excellent presentation award at the American Chemical Society (ACS) national meeting, and best papers of 2018 by the *Environmental Science and Technology Letters* Journal by ACS. Please come visit my poster and learn more about me!

4JS.26

Lucy Nandy, Visiting Postdoctoral Scholar, Assistant Professor in Chemical/Mechanical/Civil and Environmental Engineering, and Atmospheric Sciences. LUCY NANDY, University of Illinois at Urbana-Champaign

My research projects over the last decade have been a combination of aerosol science, thermodynamics, fluid mechanics, and heat-mass transfer. Currently, I study the effect of organics on particle growth by water uptake, as aerosol size distribution has impacts on atmospheric multiphase chemistry, optical properties and human-health. Current models such as PartMC-MOSAIC do not consider actual activity coefficient of organics in predicting droplet growth, yet they are important in sub-saturated conditions and cloud formation.

As a PhD student at the University of Minnesota, I advanced the perspective of particulate suspensions and multiphase phenomena, and their relevance to climate impacts. My efforts using thermodynamic modeling and droplet microfluidic experiments provided enhanced understanding of aerosol phase, gas-to-particle partitioning, and liquid-liquid morphologies. Collaboration with various research groups has aided me to find applications in finding pH and hygroscopicity of individual particles and studying morphology of real aerosol samples. Prior to doctoral studies, I have worked on industrial projects that required a heat transfer model for dynamic secondary cooling control in steel-slabs, and a mixing-model for alloy dissolution in gas-stirred steel ladle for complete homogenization. During my masters, I have worked on development of microchannel assisted cooling devices that involved image-analyzing interferometry, and on numerical simulation of evaporative processes using CFD.

My future research program will continue to develop new analytical methods with a primary focus on water, as well as mentor students with having the ability to understand science and engineering problems. My vision of developing a coherent research program merging all the skills gained from my research training will have enhanced understanding of water content in complex aqueous environments such as atmospheric aerosols.

To move forward, I will be available for a faculty position next academic year, 2020, in Chemical/Mechanical/Civil and Environmental engineering, and Atmospheric sciences any location in the United States.

4JS.27

Guangjie Zheng, Postdoc, Faculty Position. GUANGJIE ZHENG, Washington University in St. Louis

I'm Guangjie Zheng, a postdoc in Washington University in St. Louis. I'm seeking for academic faculty position in the field of atmospheric science/aerosols.

During my Ph.D. studies in Tsinghua University, China, I've been studying the extreme Beijing air pollutions. Major results include: (1) the severe winter haze was driven by stable synoptic meteorological conditions, and not by an abrupt increase in emissions; (2) secondary species, especially sulfates, were the major constituents of PM_{2.5} during this period, and (3) atmospheric chemistry during extreme hazes is characterized by weakened photochemistry versus enhanced heterogeneous reactions. Subsequently, together with my collaborators in Max-Planck Institute for Chemistry in Germany, we proposed the reactive nitrogen chemistry in aerosol water as the major sulfate formation pathway during the extreme hazes. These findings generated 5 first-author peer-reviewed papers, including 2 ESI Hot Paper (0.1%), one of which published in Science Advances.

After my Ph.D. graduation in 2016, I joined Dr. Jian Wang's group at Brookhaven National Laboratory, and moved to current affiliation with the group in 2018. During the postdoc, I've been focusing on the aerosol properties and processes in remote marine environment, based on the Aerosol and Cloud Experiments in the Eastern North Atlantic (ACE-ENA) campaign and long-term observations at the ENA site. Some of the on-going topics include: (1) key processes that drive the population of cloud condensation nuclei in remote marine boundary layer, (2) property evolutions of Canadian wildfire aerosols during the long-range transport, (3) new particle formation in remote marine environment, and (4) determining factors of size-resolved aerosol hygroscopicity in ENA.

My contract will end in Sept. 2020, and early termination is possible if needed. Please contact me through:
Cell phone: 646-301-2369
Email: gzheng@wustl.edu / guangjie.zheng@gmail.com

4JS.28

Sarah Petters, Postdoctoral Fellow: Seeking Tenure Track Position. SARAH SUDA PETERS, *University of North Carolina at Chapel Hill*

I am looking for a tenure track position at a research university in the continental United States. I am a postdoctoral fellow at the University of North Carolina at Chapel Hill, where I study the composition and partitioning of e-cigarette aerosols. My expertise includes aerosol physical chemistry, chemistry, and measurement systems. I have led the publication of research on aerosol water uptake, CCN activity, viscosity, and measurement techniques. My work has been highlighted in *Eos Trans. AGU* and won the achievement award of the Conference of Southern Graduate Schools. I was awarded the NSF Postdoctoral Fellowship (\$172k, sole PI) to study the volatility and evaporation-mediated reactions of low molecular weight organic acids and carbonyls, and the reaction kinetics of isoprene epoxydiols in aqueous mixtures. For my work I received recognition as an invited participant in the ACCESS colloquium at Brookhaven National Lab and gave invited seminars in the US and Denmark. I have collaborated with a large number of researchers in the US and Europe through participation in field campaigns (SOAS, FIN-02, FIN-03) and laboratory studies (U. Bristol, Columbia U.), some of which I am leading.

My professional activities have included committee service for AAAR, service as a panel speaker for the Air and Waste Management Association, and service as a reviewer for various manuscripts and scholarship applications.

As a student I served as instructor of record for 7 lab sections while completing a teaching certificate program, and I have taught various guest lectures for undergraduate/graduate students. I am looking forward to teaching courses in thermodynamics, physical meteorology, air pollution chemistry, scientific computing, laboratory methods, or aerosol science.

I am interested in a faculty position because I would like to continue conducting research in aerosol science, mentoring students and postdocs, and contributing to instruction.

4JS.29

Alexander J. Johnson, PhD Graduate Research Assistant, and Seeking Positions in Academia or Government. ALEXANDER JOHNSON, *Syracuse University*

My research focuses on improving our understanding of dry and wet deposition of inorganic anions, metals, and organic acids to urban surfaces. In studying dry deposition, I use surrogate surfaces to measure accumulated material and extract that material for analysis using ion chromatography (IC) and inductively coupled plasma mass spectrometry (ICP-MS). Using this approach, I am experienced with using wet-chemical methods for my research.

To study wet deposition, I measure fresh precipitation as well as stormwater runoff at intervals during a rainstorm to determine how scavenging of contaminants varies with meteorological conditions and/or chemistry. One application of this research is to determine if changes in composition of stormwater runoff from surfaces during a rainstorm reflects washoff of previously deposited material. This may enable estimates of prior dry deposition to surfaces.

I am planning to finish my PhD in May 2020 and should be available to start full-time during the summer. I am passionate about research and have plans to continue my work as a post-doc or professor in academia or as a research scientist for a national laboratory or at a government agency. I would be interested in collaborating with research scientists who have varied research interests. My geographic preference is flexible: while I am originally from the Midwest and currently located in the Northeast, I am amenable to moving to a different location in the U.S. I also am interested in moving abroad and collaborating with researchers internationally.

4JS.30

Quazi Ziaur Rasool, Postdoctoral Research Associate at University of North Carolina at Chapel Hill, PhD in Environmental Engineering from Rice University, Houston, TX. QUAZI RASOOL, *University of North Carolina at Chapel Hill*

Job type(s) of interest: Research Scientist/Postdoctoral researcher in Federal/Non-federal Research Labs or Academia, Academic faculty position

Desired area of interest: a) Atmospheric science, b) Aerosol dynamics, c) Atmosphere-biosphere interactions, d) Atmospheric/Earth system/ecosystem modeling, e) Food-Energy-Water-Air/Climate nexus, f) Air quality/climate/agricultural/public health policy

My previous research focused on mechanistic estimation of soil Nitrogen emissions in atmospheric model and their mitigation, critical to air quality and climate. My work is published in leading journals: Rasool et al., 2016 and Rasool et al., 2019 (Geoscientific Model Development) focus on modeling Soil Nitrogen emissions by integrating soil biogeochemistry in a regional-scale atmospheric model (CMAQ). Pourhashem and Rasool et al., 2017 (Environmental Science and Technology) quantifies potential public health benefits of using Biochar as a soil amendment in agriculture across US to mitigate soil NO emissions. The soil Nitrogen research was funded by NASA's Air Quality Applied Sciences Team program. For both Rasool et al., 2016 and 2019, model source codes with comprehensive and user-friendly documentation have been disseminated online to be accessed by a wide array of Earth Scientists through Oak Ridge National Laboratory's Distributed Active Archive Center for Biogeochemical Dynamics.

I have collaborated and published with federal scientists while working as a visiting scientist at National Exposure Research Laboratory, US Environmental Protection Agency (in Summer 2016) and remotely with scientists from NASA, NOAA and US Department of Agriculture.

I am currently working on incorporating mechanistic representation of phase state and separation in atmospheric aerosols that influences multiphase chemistry and secondary organic aerosols yield predicted in both regional- and global-scale atmospheric models.

Anticipated availability: August, 2020

Geographical preferences for jobs: U.S.

NOTE: Not a US citizen or permanent resident, Currently on F-1 OPT STEM extension visa

4JS.31

Dr. Kelsey Bilsback: Seeking a Faculty or National Lab Position in Air Pollution Research in the US or Europe. KELSEY BILSBACK, *Colorado State University*

I am currently a postdoctoral researcher in atmospheric science at Colorado State University (Advisor: Jeff Pierce). I am interested in using my measurement and modeling experience to conduct research focused on solving challenges related to air pollution and its effects on health and climate. Currently, questions that interest me are: How do the toxicity and optical properties of fresh smoke change depending on the source, combustion conditions, and evolution in the atmosphere? Do these changes have meaningful health or climate effects? What types of individual choices and governmental policies have the greatest health or climate benefits? What contextual factors could affect how these choices change between communities? For my postdoc (October 2018-Present), I have been using a global atmospheric chemistry model (GEOS-Chem) to quantify the health and climate effects of an energy policy that is currently being implemented in Beijing, which requires residents to transition from coal to electric heating (Bilsback et al, in prep). I plan to extend these methods to estimate the climate and health effects of other air pollution sources (e.g., anthropogenic dust). In September 2018, I defended my PhD in Mechanical Engineering from Colorado State University (Advisor: John Volckens). My PhD focused on air pollution measurements from cookstoves. I developed a novel laboratory testing protocol that became the basis for a standardized laboratory test (Bilsback et al, 2018); conducted two large-scale laboratory measurement campaigns (Bilsback et al, 2018; Bilsback et al, in review); led field campaigns in India, Uganda, Honduras, and China (Eilenberg et al, 2018); and developed a statistical methodology to estimate emissions during in-home cookstove based on laboratory data (Bilsback et al, in draft). I am currently seeking a tenure-track faculty position at a research university or a research scientist position at a national laboratory.

4JS.32

**Theresa M. Kucinski, PhD Candidate,
Postdoctoral/Government.** THERESA KUCINSKI, *The
Pennsylvania State University*

I study physical properties of submicron aerosol particles and their dependence on size, composition, and relative humidity (RH). I utilize cryogenic transmission electron microscopy to image submicron particles and I have developed a flash freeze technique that allows for the imaging of particles captured at specific RH values. Previously, I constructed a laminar flow reactor to study heterogeneous reactions between mineral dust and organic compounds to mimic atmospheric interactions. My future research interests include studying atmospherically relevant systems, combining experimental data with modeling, and designing new techniques to advance the study of atmospheric systems. My job interests include postdoctoral positions and government. The preferred geographical location is the Eastern United States but is negotiable.

4JS.33

Qi Yao, Post-doctoral Researcher, Academia/Government. QI YAO, *University of Maryland*

As both an environmental scientist and an engineer, I am intrigued with investigating different pollutants in the atmosphere, exploring potential remediation approaches, and evaluating public health risks introduced by these pollutants. Currently, my work focuses on investigating black carbon hygroscopic properties under different mixing conditions and oxidization stages, as well as developing different instrumentation-based methodology to characterize black carbon aerosols. These studies can lead to a better understanding of how black carbon contributes to droplet formation, atmospheric warming, and cloud properties. For my doctoral research, I evaluated the efficacy of vegetative environmental buffer as a cost-efficient air pollutant practice. My thesis project will ultimately contribute to the National Conservative Practice Standard (NCPS # 380 or # 420) by providing important expertise to the design and proper installation of VEBs. My goal is to continue my scientific career as a researcher specializing in the atmospheric environment. My current and previous research experiences have prepared me to be a strong technical communicator and educator promoting a broader understanding of atmospheric issues and potential solutions.

4JS.34

Julia Montoya-Aguilera, PhD Graduate Student, Government - Formation and Properties of Nitrogen-Containing Organic Compounds in Secondary Organic Aerosol (SOA). JULIA MONTOYA-AGUILERA, *University of California, Irvine*

Inorganic nitrogen contribution to particulate matter (PM) is well represented in air quality models. Missing from models is the contribution of nitrogen *organic* compounds (NOC) to PM. My PhD research explores how NOC can be produced and their effect on the amount and properties of SOA, a large component of PM. Two mechanisms for the formation of NOC in SOA were explored: (a) oxidation of a N-containing biogenic precursor (indole); (b) reactions of SOA with reduced nitrogen compounds, NH₃ and dimethyl amine (DMA), in a smog chamber. I largely examined optical properties (UV-Vis) and detailed molecular composition (PTR-ToF-MS, ToF-AMS, DART-MS) of the resulting SOA. Some findings are below:

- Indole oxidation by OH, O₃ or NO₃ efficiently produces brown SOA; indole derivatives, such as tryptanthrin, indirubin, indigo dye, and indoxyl red contribute to the visible absorption of indole SOA. The photooxidation part of this study was published (Montoya-Aguilera et al., *Atmos. Chem. Phys.*, 2017); the O₃ and NO₃ oxidation part describing our collaboration with the Dr. Yinon Rudich group is being written.
- Reactive uptake of NH₃ or DMA by low-NO_x SOA (toluene, cedrene, or limonene) does not change SOA particle mass but does change particle composition and color due to the formation of NOC, with uptake coefficients ranging from 10⁻⁵ to 10⁻³. Preliminary results were published (Montoya-Aguilera et al., ACS Symposium series, volume 1299).
- Prof. Donald Dabdub's group simulated the effect of indole SOA (Montoya-Aguilera et al., 2017) and NH₃ uptake by SOA (Horne et al., *Atmos. Environ.*, 2018; Zhu et al., *Atmos. Chem. Phys.*, 2018) on air-quality.

Overall, this PhD work highlights the novel chemistry and important properties of NOC in the atmospheric environment.

Job Type of Interest: government Geographical Preference: western U.S.

Availability: Winter 2020 (flexible)

4JS.37

Hema Ravindran, Post-doc, Desired Position – Government and Industry. HEMA RAVINDRAN, *Clarkson University*

I'm Hema and I graduated with a PhD in the field of Environmental Engineering from the top engineering institute of India, IIT Madras, in the year of 2017. My PhD dissertation was about the offline characterization of bioaerosols using DNA analyses to understand their diversity and impacts on health and climate. So, PhD was my gateway to the world of aerosols and bioaerosols. Besides gaining a significant knowledge about bioaerosols, I was able to publish some first ever reports on bioaerosols for Indian region in reputed journals like PLoS One, Scientific reports etc. I started my post-doc with Prof. Suresh Dhaniyala and Prof. Thomas Holsen last year March. As a post-doc, I first worked on passive samplers and then I started working with two grad students on two independent projects, (a) aerosol in medicine and material synthesis, and (b) low cost bioaerosol sampler development. I also work on low cost sensors to understand the air quality with a broader goal to understand aerosol-bioaerosol relationship at indoor-outdoor sites. My research interests are air quality assessment for health impacts, bioaerosol impact on human health and agriculture, and aerosol material synthesis. Besides research, I enjoy writing and this keep me going. I would love to work on areas such aerosol in threat detection etc. that would be useful to governmental organizations and industries, but I don't restrict myself to only this area.

4JS.38

Ali Akherati, Graduate Research Assistant, Mechanical Eng. Dept., Colorado State University, Air Quality Modeling/Measurements/Consultant/Policy-related Positions. ALI AKHERATI, *Colorado State University*

My primary research focus has been on understanding secondary organic aerosol (SOA) formation from a variety of different emission sources, which I have explored through modeling and analysis of field and laboratory data. Since I started my PhD program, I have worked on four different projects.

In my first project, I explored the effects of SVOCs, IVOCs, multigenerational aging, and chamber vapor wall loss artifact on SOA formation over Southern California using a chemical transport model (CTM).

In my second project with collaborators, I estimated the SOA potential from Volatile Chemical Products (VCPs), which included a variety of different emitting sources such as personal care products. The results showed that VCPs are emerging as important precursors for SOA. My collaborators and I also performed smog chamber experiments with a few VCP precursors and measured D5-siloxane, a tracer for VCPs, over the Front Range in Colorado to quantify the importance of these precursor for regional air quality.

In my third project, I investigated how ozone and PM_{2.5} would change by the year 2035 due to the shutdown of two coal-fired power plants in Colorado. The health impact assessment, conducted by our collaborators, showed a broad health benefit for Colorado residents with the highest health benefits estimated for low-income families.

In my current project, I have developed a comprehensive aerosol box model, SOM-TOMAS, which simulates size-resolved aerosol microphysics, thermodynamics, and chemical aging of different organic compounds. The model is being used to simulate biomass burning SOA formation during FIREX field and laboratory campaign.

My anticipated graduation date is Fall of 2020. After graduation, I would like to expand my existing skillset in modeling/analysis of atmospheric chemistry in areas that include, but aren't limited to, pollution, climate, policy, remote sensing, and measurement techniques.

4JS.39

Shawna Vreeke, Candidate for PhD. in Chemistry, Desired Position in Industry or Government. SHAWNA VREEKE, *Portland State University*

I am interested in the unique chemistry of aerosols. During my doctoral studies, I have gained extensive experience collecting, analyzing and evaluating aerosol chemistry. My main focus is on electronic cigarette aerosol toxins. For this study, I have employed EPA standard analytical methods in addition to developing and/or validating techniques including quantitative GCMS and non-destructive quantitative NMR. As a result, I am interested in opportunities to continue to develop novel analytical methods. Additionally, I am interested in the fundamental chemistry of aerosols. My training as an organic chemist has enabled me to elucidate the reaction pathways of aerosol product formation. This includes both benchtop and theoretical work. For example, I have derived a mathematical model to predict toxic aldehyde and related degradant levels in e-cigarette aerosols. I have been trained in the analysis of large data sets via statistical programs such as STATA and SAS as part of a certificate program I completed in the use of PATH (Population Assessment of Tobacco and Health) data. In addition to e-cigarettes, I am interested in related investigations such as the study of the reactions of indoor air with surfaces.

In closing, my ongoing interest in aerosol science coupled with my classical training in organic chemistry will allow me to be a significant contributor to industrial or government projects involving aerosol science. My thesis defense is in November of 2019. I will be available to begin work immediately after earning my PhD. I would prefer to work in Oregon or relocate to other western states of the U.S.

4JS.40

Aditya Sinha, Graduate Student Researcher, Industry. ADITYA SINHA, *North Carolina State University*

The research question my work addresses is how atmospheric pollutants and their associated properties transform in the atmosphere. Secondary organic aerosol (SOA) are air pollutants produced through complex interactions of sunlight and volatile organic compounds (VOCs). SOA form a major component of particulate matter and so understanding its properties are important. I have focused on SOA from cookstove emissions, which approximately 3 billion people use for their daily needs. To study SOA, I employed the use of an oxidation flow reactor (OFR) – which simulates days of atmospheric aging on the timescale of minutes. Upon conducting these experiments in conjunction with various supervised and unsupervised statistical learning techniques, I gained insight into how cookstoves of different efficiencies and fuel types affect the physical and chemical properties of SOA. Through this, I built on my analytical skills developed during my Master's at Carnegie Mellon University on working on mathematical models of kinetic parameters.

In addition to conducting laboratory controlled experiments, I have also worked on characterizing SOA in a real-world setting. Field monitoring efforts have consistently shown a clear distinction between in-field performance of cookstoves and that measured in standardized lab tests. To address this disparity, in the context of SOA from cookstoves, I conducted an experimental campaign in a 'quasi-field' setting in Mexico to observe differences in SOA in the two environments. During this campaign, I focused on the application of low-cost sensors to characterize SOA in favor of complex and immobile instrumentation.

I am currently working on the application of deconvolution algorithms in identifying organic species from chromatograms in collaboration with the EPA. In addressing these research questions I have picked up strong transferable data analytical skills (in R, Python, Igor) along with significant experimentation experience. Upon graduation in April 2020, I hope to use these data analysis skills in an industry based setting (no geographical preference).

4JS.41

Bo Yang, Ph. D. Candidate, Academia/Industry opportunities in Environmental/Mechanical Engineering. BO YANG, *Cornell University*

I have a diverse research background and I am looking for academic/industry opportunities for solving environmental/mechanical engineering challenges.

My current project is using computational fluid dynamics (CFD) to parameterize the near-source air quality impact from distributed generation (DG) and highway traffic emission sources. For the electricity generation emission sources, I am working closely with USEPA on the building downwash modeling. I published three journal papers about the turbulent reactive plume from a central coal-fired powerplant, a simple cycle gas turbine, and a combined heat and power distributed generation facility. These papers set up a good foundation for the current project. I am also working on a project of assessing air quality improvement of using a combined cooling, heat, and power facility for a large wholesale market. For the highway traffic emission source, the current Gaussian-based dispersion models treat the highway region as a well-mixed zone. I published one paper on *Environmental Science & Technology* to show the direct evidence that from the vehicle tailpipe to the highway curbside, a significant part of NO₂ was transformed from NO by ambient O₃. The on-going work is to parameterize the on-road NO₂/NO_x ratio and provide a better initial NO₂/NO_x ratio condition for the dispersion models. As for the field and wind tunnel measurements, I led the mobile measurement of the residential wood-burning smoke in downtown Ithaca, NY. I joined the real-time emission measurement of a biomass boiler. I designed the wind tunnel tests for the on-road chasing measurement of highway vehicle emissions. In addition, I have research experience in the automotive industry. I led an HVAC system design for a passenger car. I led and joined several aerodynamic design projects from OEMs.

4JS.42

Alison Fankhauser, Ph.D. Student and Desired Post Doc or Industry Research Position. ALISON FANKHAUSER, *Columbia University*

Secondary organic aerosol (SOA) is a significant component of ambient tropospheric aerosol and a comprehensive understanding of its sources and sinks is imperative for determining the effect on atmospheric processes, air quality and climate. SOA formation and growth involve complex and varied chemical and physical processes, and despite substantial advancements over the past decade, the SOA budget has not been closed. This work explores four distinct projects to address the sources and sinks of SOA in aqueous aerosol particles: 1) the photochemical aging of an isoprene SOA tracer, 2-methyltetrols; 2) the detailed speciation and formation rates of IEPOX-derived SOA using GAMMA; 3) the extent of photoactivator chemistry under ambient conditions, a potential source of organic aerosol mass via direct oxidation of volatile organic compounds or generation of oxidants in the particle phase; and 4) the effect of bacterial metabolism on organic aerosol content. The results of this work will yield an improved understanding of atmospheric aerosol chemistry with implications for air quality and climate.

I am a Chemical Engineering Ph.D. student at Columbia University with substantial laboratory experience as well as a modeling background. With an anticipated defense by the end of 2019, I seek a post doc or industry position to broaden my knowledge in the field of atmospheric aerosols. In particular, I would like my future work to have more direct policy relevance and to apply either my instrumental experience to fieldwork or my coding skills to a multidimensional model. Ideally, I want to relocate to the West Coast or remain on the East Coast. I hope to continue growing as a diligent scientist within our aerosol research community.

4JS.43

Huang Zhang, Postdoctoral Scholar(Ph.D), Faculty & Industry, CA & OR & WA. HUANG ZHANG, *Washington University in St Louis*

I am Huang Zhang, now as a postdoctoral scholar in Dr. Pratim Biswas' lab from Washington University in St. Louis.

I got my Ph.D (2015) from Tsinghua University, China. My research interest during my Ph.D work was gas-liquid two phase flow modeling, which is helpful in optimizing the design of moisture separator (or droplet eliminator) in Chemical/Nuclear/Environmental Engineering. Then I stayed in Tsinghua University for accomplishing 2 years postdoctoral work. My interest jumped to aerosol modeling to understand the performance of Electrostatic Precipitator (ESP). In 2017, I came to Washington University in St. Louis (WUSTL) to continue my research on aerosol modeling. In WUSTL, my aerosol modeling work is used to understand the performance of aerosol instrument, like Differential Mobility Analyzer (DMA). Also, I have a master degree in computer science from Tsinghua University. Thus, my practical knowledge of computer science lets me be able to participate in a project on analyzing air quality data by Machine Learning approaches.

I am looking for a faculty position or research engineer in industry.

My contract will end with WUSTL on Aug 31, 2020.

My geographical preference is on the Western coast. California, Washington or Oregon State is good for me.

My contact information is:
Cell phone: 858-732-2930
Email: huangzhang@wustl.edu /
chengzhuanghuang87@gmail.com

4JS.44

Yangyang Zou, PhD candidate in the Ohio State University / Civil Engineering (Environmental Engineering) / Industry, Postdoc and Faculty Position. YANGYANG ZOU, *The Ohio State University*

Yangyang Zou earned her bachelor's degree in Architectural Engineering at Beijing University of Civil Engineering and Architecture. She then worked as an HVAC engineer in Chinese Academic of Science for two years. She finished an MS degree in Environmental Engineering at Texas A&M University – Kingsville, working as a research assistant for two and half years on projects related to the nano-particle filtration mechanism and modeling. She began her PhD study in Civil Engineering (following the Environmental track) at The Ohio State University in January 2016. Her current research focuses on the application of low-cost air quality sensors in real-world settings (including both gas and particle sensors). Her research projects include 1) identifying spatial variation of air pollution over urban roadways using an air-quality-sensor-equipped transit bus; 2) facilitating the use of low-cost air quality sensors by citizen scientists (high school students) to provide reliable air quality data within micro-environments; and 3) evaluating low-cost particle sensors for indoor air quality monitoring and smart building systems. Her position at OSU has mostly been a graduate research assistant, but she also worked as a graduate teaching assistant for one semester where her roles included holding office hours, grading exams, facilitating laboratory exercises, and serving as a guest lecturer while her advisor attended AAAR. Her projected graduation date is May 2020.

Following the completion of her doctoral degree, Yangyang is open to positions in both industry and academia. She is a determined person who wants to continue to work with air quality monitoring technology. She believes that improving air quality is essential to a health life. Air quality monitoring became smarter with rapid developing technology and big data solutions. Since air quality sensor is still an emerging technology, she desires to dedicate her efforts to this field.

4JS.45

Mara Otero-Fernández, PhD Student, Bio Science Area. MARA OTERO-FERNANDEZ, *University of Bristol*

Technological advances in the biosciences continue to open new growth opportunities to confront challenges in the future. Personally, I believe an enormous potential for the advantage of society lies in the Life Sciences whose applications in health, agriculture, medicine, and the pharmaceutical and food industries are helpful in improving the quality and standard of life. I'm motivated to contribute to these ongoing innovations and feel that my background and research experience are in line with my professional interests.

During my studies at the University of Santiago de Compostela (Spain), my focus was on Analytical and Environmental Chemistry and I was also especially involved in R&D in the area of toxicology. In my research thesis, I played a crucial role in the development of a robust methodology to quantify the presence of narcotics in biological samples for toxicological application. These studies have been published in *Analytica Chimica Acta* (Otero-Fernández et al., 2013).

Further to my academic studies, I have industrial experience working as a production chemist within the ceramics industry, performing quality control of materials involved in manufacturing processes.

Afterward, I acquired funding for a short-term research project by the Lifelong Learning Programme of the European Commission to work in the lab of Prof. Jonathan Reid at the University of Bristol. I had the pleasure to collaborate in the initial development of a novel approach named CELEBS to interconnect the complexity of aerosol dynamics with bioaerosol longevity, aiming to fully understand the mechanisms of airborne transmission. This research opportunity led into a research assistant position and subsequently in my current Ph.D. project, contributing to a new partnership between DSTL and Bristol University. These studies have been published in the *Royal Society Interface* (Otero-Fernandez et al., 2019).

Upon the completion of my Ph.D. in May 2020, I would relish the opportunity to delve deep into these subjects with a postdoctoral or industrial position where my work could contribute to a better understanding of the fields of airborne disease dynamics and treatment.

4JS.46

Maksim Islam, 3rd Year PhD student at NC State University, Research & Development (R & D). MOHAMMAD MAKSIMUL ISLAM, *North Carolina State University*

My name is Maksim Islam, a 3rd year Ph.D. student in the department of Civil, Construction and Environmental Engineering at North Carolina State University (NCSU).

What drives me to work in the field of environmental engineering, and air quality, in particular, is largely my experience at home in Bangladesh. There, the black smoke curls up from brick kilns and the smog shrouds the sky of Dhaka (the capital city), with its ant-like army of vehicles clogging up the streets. My undergraduate research (conducted in Bangladesh) allowed me to elucidate dynamic interactions between meteorology, pollution sources, and the fates of atmospheric aerosols, with the ultimate goal of improving air quality and reducing human exposures to air pollutants. Later, after witnessing the unbearable sufferings of the people living in coastal Bangladesh- due to a scarcity of potable water- I was drawn to rainwater harvesting research, the focus of my M.Sc. During this time, I applied my programming and modeling skills to develop design curves for storage tank sizing based on reliability concepts. My strong mathematical background always encourages me to blend mathematical concepts and programming skills in my field of interest.

I began my Ph.D. research work at NCSU on air pollutant emissions and indoor air quality impacts of cookstoves. Globally over 3 billion people use biomass stove, and the emissions from it are associated with 4 million premature death each year. With a dream to change this scenario, I work as a part of a large interdisciplinary team to analyze data from a multi-year cookstove intervention project in rural India. My prime foci are emissions from cookstoves and their subsequent influence on indoor air quality, which interact with stove choice, stove adoption and diffusion, and fuel use.

I am planning to defend my Ph.D. dissertation in summer of 2020. I am interested in both academia and industry, and dream of attaining a postdoctoral research position that focuses on the energy-emission-indoor air-policy nexus.

4JS.47

Tofigh Sayahi, Chemical Engineering PhD Student, Chemical Engineering. TOFIGH SAYAHI, *University of Utah*

My research interests include understanding the performance of and effectively deploying low-cost air-quality sensors in for a variety of applications. During my PhD, I have developed several skills including data analytics, computational fluid dynamics, and field testing. My achievements including designing and evaluating a cost-effective aerosol calibration chamber, capable of providing uniformly distributed particle concentrations to eight sensors and a reference instrument for laboratory evaluation of low-cost sensors. I have also been developing strategies, including machine learning, for field calibration of low-cost particulate matter and metal oxide ozone sensors. I am part of an interdisciplinary team who developed the AQandU infrastructure, a dynamic network of over 100 low-cost sensors that provides an estimate of PM_{2.5} levels throughout the Salt Lake Valley. With more than 3 years' experience as a teacher assistant, I am also adept in motivating, instructing and supporting students.

I will be available in April 2020. I am looking for a position that will allow me to build on my skills with low-cost sensors such as a postdoc or an industrial position. My geographical preference for a job is the United States of America.

4JS.48

Meet Hanyang Li, Ph.D. Candidate Who is Seeking a Research Job in Atmospheric Science. HANYANG LI, *The Ohio State University*

I am a Ph.D. candidate in Civil Engineering with an emphasis in atmospheric aerosols at The Ohio State University. I hold a MS (2016) in Mechanical Engineering from University of Colorado Boulder. I expect to complete my Ph.D. by May 2020 (if not sooner) and look forward to becoming a research scientist in the field of atmospheric science (e.g., a postdoc in either industry or academia). My primary career goal is to conduct high-quality and independent research with the help of advanced statistical or machine learning methods (such as deep neural networks).

The primary focus of my current research is constraining uncertainties in light absorption and black carbon (BC) measurements. Accordingly, my research objectives are to: 1). Quantify potential differences among the BC measurements and examine any systematic relationships between aerosol chemical/optical properties and observed differences; 2). Develop a generic correction algorithm for any filter-based absorption photometer to constrain BC estimates between different instruments; and 3). Predict BC optical properties utilizing deep learning approaches.

To meet these objectives, I am conducting both experimental studies (laboratory and field experiments using several aerosol-related instruments) and computational analyses (such as statistics and machine learning using Igor Pro, R, Python, and MATLAB). Specifically, I have worked on the following research tasks: 1). Conducting field experiments and operating instrumentation at U.S. Forest Service Fire Sciences Laboratory; 2). Analyzing the BC samples in the laboratory at OSU campus; 3). Using a set of statistical tools to understand the data; and 4). Developing artificial neural networks and other statistical models to constrain measurement uncertainties.

Overall, I enjoy addressing challenging research questions via creative and critical thinking. I believe my graduate education and research experiences would contribute to my future success in the professional career as a scientist in the field of atmospheric science.

4JS.49

Jiayu Li, PhD/Postdoc/Low-cost Sensor and Aerosol Engineering. JIAYU LI, *Washington University in St Louis*

My Ph.D. work is related to design, calibration, and application of low-cost PM sensors. The new trends of PM concentration measurement are personalized portable devices for individual customers and networking of large quantity sensors to meet the demand of Big Data. Therefore, low-cost PM sensors have been studied extensively due to their price advantage and compact size. Multiple types of low-cost PM sensors and monitors were calibrated against reference instruments. All these units demonstrated high linearity against reference instruments with high R2 values for different types of aerosols over a wide range of concentration levels. Optical characterization of low-cost PM sensors (ensemble measurement) was conducted by combining experimental results with Mie scattering theory. The reasons for their dependence on the PM composition and size distribution were studied. To get rid of the influence of the refractive index, we propose a new design of a multi-wavelength sensor with a robust data inversion routine to estimate the PM size distribution and refractive index simultaneously. We have deployed sensor network in a woodworking shop for spatiotemporal pollution mapping. Data collected by the networked 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. Furthermore, for the outdoor environment, data reported by low-cost sensors were compared against satellite data. The integration of data sets was also a way to enhance the overall data quality and accuracy of these low-cost sensors. The maps created from these three data sources demonstrate an approximate 30-fold synergistic improvement in the spatial resolution of PM mapping, with minimal bias. This method will greatly assist the validation of PM transport models and enhance the accuracy of exposure estimations.

4JS.50

Collisional Growth, Charging and Measurement of Molecular Clusters to Sub-10 nm Particles in High Temperature Flame Environment. GIRISH SHARMA, Rajan K. Chakrabarty, Pratim Biswas, *Washington University in St Louis*

It is important to understand the early stages of particle formation and growth in high temperature combustion systems for both nanoparticle synthesis and environmental applications. According to conventional understanding, at high flame temperatures, the particles collide with each other and coagulate to form larger particles. Contrary to this understanding, our previous work shows that during the early stages of particle formation and growth (< 2 nm), charged particle fraction is very high (> 95%), suggesting that in addition to neutral particle interactions, there are charged particle, and ion-particle interactions as well.

My PhD work can be divided into three major chapters viz. collisional growth, measurement, and charging of sub-10 nm particles. First, collisional growth of titania nanoparticles is studied at moderately high temperatures from 400 – 800 C; and it was found that the collisional growth rate is found to be higher than predicted by kinetic theory of gases. Experiments show that there is higher enhancement in the collisional growth as compared to theories based on Hamaker constant. Following this, molecular dynamics simulations are performed to understand the interatomic forces that lead to this enhancement in collisional growth.

Second, the commonly used equipment for sub 2 nm particle measurement, half-mini differential mobility analyzer is characterized. The working section of the half-mini DMA is simulated using commercial software COMSOL. Comparison of the simulated transfer function with existing models from Knutson-Whitby and Stolzenburg is also elucidated. It is found that the former model overestimates the resolution; whereas the latter is close to the simulation results for aerosol flow to sheath flow above 0.067. This work provides a useful method to study the flow regimes and transfer function of a high flow DMA.

Third, the well characterized half-mini DMA is used to study the early stages of particle formation and growth mechanism for titania nanoparticle synthesis from TTIP precursor in a flame aerosol reactor as well as soot nanoparticles from McKenna burner. The insights from the total and charged particle size distribution, starting from molecular clusters to sub-10 nm particle size provides new insights into the particle formation and growth mechanism. To further understand the role played by charge, a model for simultaneous charging and coagulation is developed using the method of moments.

4JS.51

Meet the Job Seekers Poster Session - Qing Ye. QING YE, *Massachusetts Institute of Technology*

I received a joint Ph.D. degree in Chemistry and Engineering and Public Policy from Carnegie Mellon University in 2019. In my Ph.D. study, I worked on using state-of-the-art analytical techniques to measure physical and chemical properties of organic aerosols in laboratories in order to understand key processes governing the fate of organic aerosols. I used both the smog chambers at Carnegie Mellon and the CLOUD chamber at CERN to study atmospheric new-particle formation as well as gas-particle partitioning of atmospheric organic vapors. I also extended my laboratory studies to field measurements and characterized the chemical evolution of organic aerosols and human exposure to different sources of aerosols in an urban environment. I also have a strong environmental policy hoping to work at the interface of science and society in the long run.

I am currently a postdoc associate at MIT working on understanding the lifecycles of reactive nitrogen species in the atmosphere. I am interested in learning the complex interplays between naturally emitted reactive compounds and anthropogenic pollutants. I am seeking for international environmental-related jobs in academia, industry and government. Tentative starting time is in 2020 or 2021.

4JS.52

Meet the Job Seeker: Vikram Pratap. VIKRAM PRATAP,
University of Maryland, Baltimore County

I am currently appointed as a postdoctoral research associate at the University of Maryland, Baltimore County in Dr. Hennigan's lab. My work focuses on studying the impact of ammonia on brown carbon formation in ambient aerosol. As part of my work at UMBC, I developed skills in using, Particle-into liquid sampler (PILS), total organic carbon (TOC) analyzer, Liquid waveguide capillary cell (LWCC), PILS-IC, benchtop UV-vis spectrometer, and other laboratory activities.

In my Ph.D. work, I investigated the lifetime of wood smoke molecular marker (levoglucosan) in winter conditions in context to the use of wood for space heating purpose. I conducted fresh wood smoke photochemistry experiments at temperatures ranging from -15oC to 15oC. The work was funded by an external agency through a two-year project. In this limited time, I single-handedly established an entirely new outdoor chamber experiment facility to conduct my experiments, which included calibration, installation and/or construction of a 6 m3 smog chamber, a UV light panel system, a wood stove, compressed air system, wood smoke analyzer, SMPS, NOx analyzer, O3 analyzer.

I also mentored many undergraduate and graduate students during my Masters, Ph.D. and postdoctoral work.

Additionally, I have 10 years of wide industrial work experience ranging from material research, chemical research to process engineering in defense, chemical and food industry. In this span of time, I acquired several research and engineering skills which I am confident will be useful in conducting my duties.

I will be available from February 2020 for opportunities in the industry, government or academic institutions, that can take advantage of my broad skills in research, atmospheric science, and chemical and process engineering. I do not have any location preference and would be happy to relocate for the job requirements.

4JS.53

Patricio Piedra, Postdoctoral Physicist Seeking Permanent or Permanent-prospective Job as Researcher/Data-Analyst.
PATRICIO PIEDRA, *U.S. Army Research Laboratory*

In the broadest sense, I am interested in electromagnetic waves interacting with matter and retrieving information that can be used to characterize such matter remotely. Some examples of applications include aerosol remote sensing, characterization, and classification. In recent years, I have experimented with optical tweezers for trapping single aerosols and characterizing them using elastic and/or inelastic (i.e., Raman and Fluorescence) spectroscopy. I have recently treated electromagnetic scattering as a computational, big-data, machine-learning problem, and I have successfully demonstrated that Machine Learning can be used to classify the morphologies of aerosols from scattering datasets with great accuracy. I am currently researching the mechanisms of how Machine Learning finds patterns in such electromagnetic scattering datasets. These findings should pave the way to improved capabilities to detect and characterize trace aerosol. During my dissertation, I studied how particles scatter electromagnetic waves in the forward or backward direction and how this dependence affects the efficiency of solar modules deposited by particles. The papers I wrote during this period have been of strong interest to DOE audiences that study solar panel efficiency. Furthermore, during my M.S. in Physics education, I studied how we can model and classify aerosol by the degree of linear polarization of electromagnetic scattering. My dream position would be an academic research position in the West Coast, particularly California due to family; however, for the correct opportunity, I am willing to move anywhere in the U.S. Please note that I am looking for a permanent position, but I would accept a temporary/postdoctoral position provided that there are good avenues of reaching permanence. I have a skillset that includes large-dataset statistical/numerical modeling, laboratory skills for spectroscopy and optical table laser-spectroscopy, and academic writing and presentation.

4JS.54

Use of Breath-Borne Biomarkers for in Vivo Monitoring Air Toxicity. HAOXUAN CHEN, Xinyue Li, Maosheng Yao, *Peking University*

Many substances in the air are harmful to human health, such as PM, ozone, bioaerosols etc. Therefore, human are confronting synthetical threats from the air and the real-time monitoring of air toxicity is crucial and necessary, which however is a long-standing challenge in the field. The present practice are usually performed by online monitoring single or several already-known toxicants, which fails to provide overall information about the air safety. Besides, toxicology studies are most offline, thus being not able to track the in situ responses of animals or humans to airborne toxicants exposure.

Recently, exhaled breath is increasingly being used as a noninvasive biomarker in environmental health studies. In addition to its non-invasive property, the exhaled breath can be continuously obtained which makes it possible to real-time reflect air toxicity. Here, we reported a system called dLABer that allows us to real-time monitor the breath-borne biomarkers. The system integrates living animals, breath sampling and detection module. To test the dLABer, rats exposed to different kinds of air pollutants and toxicants were used as the subjects. Our data showed that the dLABer were able to online report different types of biomarkers in exhaled breath of rats after exposure to different toxicants. Based on breath-borne biomarker levels, the system can not only distinguish the different toxicity of PM collected from different global cities, but can also served as a direct monitor of the overall air toxicity. In the future, the system can be used to monitor the biomarkers in many other scenarios. This work leads to a frontier method that is expected to pioneer the air toxicity monitoring as well as many breath-borne disease diagnosis and studies.

4JS.55

Chih-Hsiang Chien, PhD, PostDoc/Faculty/Engineer, Academic/National Lab/Industry. CHIH-HSIANG CHIEN, *University of Florida*

My Ph.D. dissertation focused on the development of a novel and low-cost personal sampler to monitor workers' indoor exposure to sulfuric acid mists and sulfur dioxide gas in the occupational setting. I participated in a project to mitigate the particle soiling on the solar panel by alternating strong electric field. One current project is to apply a portable analytical method for on-the-spot qualification of respirable crystalline silica in construction industry to promote early exposure monitoring. Another current project is to design an in-stack sampler in saturated or droplet-laden stacks as an EPA Other Test Method. I apply computational fluid dynamics to evaluate and optimize the prototype. I have experience on aerosol generation, field measurement/sampling, chemical analysis such as ion chromatography, and computation fluent dynamics (Fluent & OpenFOAM). I am a team player and I have rich experiences working collaboratively with the consortium of construction safety and health, phosphate research institute, EPA, paper industries, and petroleum sector. My research interest includes engineering applications to environmental monitoring/mitigation in the occupational setting, air pollution control, and aerosol/gas instrumentation design. I am currently seeking for postdoctoral/engineer position in university/national labs/industry. No special geographical preferences.

4JS.56

Time-resolved Spread of Antibiotic Resistance Genes in Highly Polluted Air. TING ZHANG, Maosheng Yao, *Peking University*

Antibiotic resistance genes (ARGs) have emerged as a global health concern. A large volume of work has already been devoted to ARGs in aquatic ecosystems. However, ARG dispersal patterns in air remain to be largely unknown despite of its greater role in transmission. This work aims to investigate time-resolved airborne spread of ARGs and their corresponding subtype bacterial carriers in highly polluted air. Time-resolved air samples were collected using a high volume sampler every 4 h continuously during low and high PM_{2.5} pollution times in Beijing. All air samples were subjected to 16S rRNA sequence analysis for 39 ARG subtypes. Pure culturable bacterial isolates from Beijing and Shijiazhuang were shotgun sequenced for species identification and also subjected to high throughput ARG subtype detection. ARG and its subtype relative abundances in the air were observed to spread widely both day and night, and the blaTEM gene was found to lead the ARG abundance. For an early morning time, the multi-drug resistant NDM-1 gene was detected up to 30% of total ARG abundance in highly polluted air. Identified as a major NDM-1 and vanB gene carrier, *Bacillus halotolerans* were also shown to disseminate more ARG subtypes. On another front, tnpA and int11 were shown to vary greatly in abundance, while the sul3 gene was found widespread among the culturable *Bacillus* isolates in the air. PCA showed different gene co-occurrence networks for different PM_{2.5} pollution episodes, e.g., tnpA and int11 for gene transfer and integration, respectively, were found more abundant for the high PM_{2.5} pollution episode. This study highlights a serious yet previously unidentified public health threat from time-resolved airborne spread of ARGs. Further work is urgently warranted to track the sources of ARGs for their optimized control during high PM_{2.5} pollution episodes.

4JS.57

Dishant Khatri, Final Year PhD Student, Combustion and Aerosols, Looking for Industry Job. DISHANT KHATRI, *Washington University in St. Louis*

I am currently a graduate student in department of Energy, Environmental, and Chemical Engineering at Washington University in St. Louis. My Ph.D. research is focused on broad topics of combustion and aerosol engineering. My expertise is on designing and commissioning of lab and pilot scale combustion systems, developing aerosol sampling systems for high pressure and high temperature combustion environments, measuring solid particles temperature using two-color pyrometry, utilizing high speed videography for non-intrusive flame measurements and flame design and analysis.

I am anticipated to be available after spring 2020. I am interested to work in the role of research and development engineer/ process engineer in an industry.

I am open to any geographical location but east coast or west coast are preferred.

4JS.58

Mehdi A. Torkmahalleh, Assistant Professor at Nazarbayev University, Seeking a Faculty Position at the Rank of Assistant/Associate Professor. MEHDI AMOUEI
TORKMAHALLEH, *Chemical and Aerosol Research Team, Nazarbayev University*

I am currently an assistant professor in Chemical and Materials Engineering at Nazarbayev University, Kazakhstan and have more than 6 years of experiences as an assistant professor and published more than 30 papers (with H-index 11 in Scopus). I published more than 15 papers in prestigious journals including Q1 ranking in 2017-2018. I have also several teaching experiences and grant writing and served in different departmental and school committees. So far, I could obtain more than 150K USD grant. The cooking in residential or commercial kitchens and diesel engine emissions in highway and city traffic zones are the major producers of the UFPs, indoors and outdoors, respectively. Some epidemiological studies revealed associations between exposure to cooking fumes and diesel engine exhaust, and lung cancer. Several clinical exposure studies are available in the literature that investigated the effect of acute exposure to cooking and traffic fumes on human health. Several animal studies conducted in the literature addressed the translocation of different types of nanoparticles to the extra-pulmonary organs such as cardiovascular and nervous systems, but yet discrepancies exist in the literature with respect to animal studies. My next five years research goal is to study the impact of UFPs from different sources particularly cooking and traffic on human brain through clinical, animal and in-vitro studies to better understand the underlying mechanisms for the translocation of the nanoparticles to human brain. The brain activities during and after exposure to UFPs are compared with what has been observed for neurodegenerative diseases such as Alzheimer and Parkinson. My recent and preliminary studies (*Neurotoxicology* 2019. 74:149-161), showed that exposure to aerosol from cooking using electric stove changes the human brain wave pattern. Please join my talk at Session 3 Room A 106: Tuesday, 4:15 PM - 4:30 PM Paper Number: 3.AD.4.

4JS.60

Nethmi Kasthuriarachchi, PhD candidate, Postdoctoral Researcher, Europe. NETHMI KASTHURIARACHCHI, *National University of Singapore*

Light absorbing carbonaceous aerosols are a topic of great interest within the aerosol research community due to its direct and indirect effects on the global climate. Particularly, the study of brown carbon (BrC), the fraction of organics that absorb light in the near ultra violet and visible wavelength region, has been gaining traction since the last decade, primarily due to its prominent light absorbing properties and its potential influence on the reduction of atmospheric oxidants.

My current studies focus on the analysis of long-term ambient measurement of urban aerosols to identify potential sources of urban BrC and to quantify their source-specific optical properties based on measurements from a seven-wavelength Aethalometer, incorporated with chemical characterization data from a high resolution-aerosol mass spectrometer (HR-AMS). HR-AMS is used to further understand the chemical composition of the BrC chromophores contributing to light absorption. Another part of my research includes laboratory work for investigating the effects of relative humidity (RH) on the formation of secondary BrC by simulation of atmospheric droplet evaporation process with model reaction systems. This study revealed, for the first time, that BrC formation varies as a function of RH and the observations were further generalized for more complex secondary aerosol mixtures produced using a potential aerosol mass (PAM) reactor.

As a final year PhD candidate in the Department of Civil and Environmental Engineering at the National University of Singapore I expect to complete my degree by July, 2020 and will be available for any postdoctoral research opportunities immediately afterwards (preferably, in the European region). I am interested in carrying out both laboratory and field work in projects that focus on the formation and the chemical/physical processing of atmospheric aerosols, where my experience with the aforementioned instruments and handling of large data sets would be utilized.

4JS.62

William G. Tsui, Ph.D. Candidate and Desired Area: Government or Industry. WILLIAM TSUI, *Columbia University*

I am a Ph.D. candidate at Columbia University in the Department of Chemical Engineering expected to graduate by May 2020. Currently, I am primarily looking for positions in government or in industry with a slight preference for the northeast U.S., although geographical location is certainly not a deal-breaker for me.

My Ph.D. work consists of two main projects: (1) modeling aqueous secondary organic aerosol (SOA) production from photosensitizers, and (2) examining the impact of aerosol-cloud cycling on aqueous SOA formation. Both of these projects are modeled using GAMMA (Gas-Aerosol Model for Mechanism Analysis), an atmospheric photochemical box model developed by the McNeill group with coupled gas and detailed aqueous phase chemistry. In the first project, laboratory studies of imidazoles and humic-like substances acting as photosensitizers in aqueous aerosols were modeled in GAMMA and scaled to atmospheric conditions to consider their importance in ambient processes. In the second project, isoprene epoxydiol SOA and organic acid formation in both cloud water and aqueous aerosol was quantified in GAMMA using ambient conditions from Whiteface Mountain and the effect of cycling between the two aqueous regimes on SOA production modeled. I hope to expand my knowledge of atmospheric models and to apply my experience in computational modeling of atmospheric aerosols to large-scale and multidimensional models as I begin my career in the aerosol field.

4JS.63

Sukrant Dhawan, Graduate Student Researcher, Seeking Internship Position in Industry. SUKRANT DHAWAN, *Washington University in St Louis*

I am currently a graduate student in the department of Energy, Environmental, and Chemical Engineering at Washington University in St. Louis. I am working under the guidance of Prof. Pratim Biswas. My Ph.D. research is focused on understanding the formation of nanomaterials from the droplet to particle via the aerosol route. I am working on modeling different dynamics taking place within the droplet that can influence the synthesized particle morphology. I am also doing experiments to understand the charging behavior of particles which are synthesized using spray assisted flame aerosol reactor and plasma reactor.

My anticipated graduation is May 2021. I am looking for an internship position in the role of a research engineer in industry.

I am open to any geographical location.

My contact information is: sukrant@wustl.edu

4JS.64

Weihan Peng, Ph.D. Candidate in Chemical and Environmental Engineering at University of California, Riverside, Seeking for Industry/ Consulting/ Government Opportunities in Air Quality Field. WEIHAN PENG, *University of California, Riverside*

My research primarily focuses on the understanding of NO_x effects on Secondary organic aerosol (SOA) formation to improve the prediction accuracy on SOA of air quality models, with the use of smog chamber and SAPRC gas-phase mechanism. I have developed novel methodologies simulating real-time NO_x conditions in smog chamber and SAPRC, which provides more representative SOA parameters and better sensitivity to NO_x conditions on SOA prediction. I have also studied effects of ethanol content in fuels and drive condition on SOA from gasoline direct injection (GDI) vehicles using a mobile environmental chamber.

In addition to SOA, I have also conducted several field studies on primary emission from marine vessels. I have studied the impacts, which includes air quality, global warming and health risk assessment, of switching from traditional diesel fuel to natural gas on marine vessel, one of the first comprehensive studies on natural gas vessel.

I'm planning to graduate by June 2020 and currently seeking for job opportunities in industry, consulting or government after I graduate. (No geographical preference).

4JS.65

Amirhosein Mousavi, 4th-Year PhD Candidate, Post Doc/Industry Research Position. AMIRHOSEIN MOUSAVI, *University of Southern California*

Bio:

Amir has a **BSc** in Chemical engineering from the Sharif University of Technology and **MS** in Environmental Engineering from the University of Southern California. He is currently a 4th year **Ph.D. candidate** at the University of Southern California working with Prof. Constantinos Sioutas where he has conducted series (*11 peer-reviewed Journal publications*) of long term particulate matter (PM), PM-bound species and health marker source apportionment studies in different areas of the world to understand the spatiotemporal variation of PM relatable to aerosol chemistry and crucial for policymakers and forecasting.

Interest topics:

Atmospheric Science, Remote sensing in air quality, Air pollution exposure, PM associated Health effects.

Skills:*- Data handling:*

hands-on experience with different programming languages (i.e., R and python), source apportionment models (i.e., PMF, UNIMAX, CMB) and statistical analysis tools (SPSS).

- Remote sensing:

NASA health and air quality remote sensing program certificate and satellite data processing, GIS visualization for air quality data.

- Experiment design:

long-term air pollution measurement field campaigns, Set up and operate a range of air quality instrumentation— from cascade impactors to SMPS and OPS.

- In-vivo and in-vitro air pollution exposure:

Several real-time mice exposure campaigns as well as in vitro sample collection in collaboration with health perspective experts.

Job interest:

Postdoc/industry/Consulting research positions.

Geographical preference:

California is a plus!

Preferred start date:

May 2020

Contact:

amousavi@usc.edu

5AC.1

Hydroxyl Radicals from Isoprene Hydroxy Hydroperoxide (ISOPOOH) Decomposition Induced by Irons in Water. TING FANG, Pascale Lakey, Jean Rivera-Rios, Frank Keutsch, Manabu Shiraiwa, *University of California, Irvine*

The hydroxyl radical (OH) is one of the most important oxidants in the atmosphere. It reacts both in the gas phase and in clouds and it is involved in the secondary processing of the majority of organic species. It is also a key reactive oxygen species that play a crucial role in air quality and human health. Sources of OH like ozone (O₃) and hydrogen peroxide (H₂O₂) are well studied but the kinetics and formation mechanisms of OH radicals by organic compounds are not well understood. In the present study, the isoprene oxidation product, isoprene hydroxy hydroperoxide (ISOPOOH), was synthesized in high purity to investigate its potential to form OH radicals in the presence of inorganic iron(II) and iron(III). Using electron paramagnetic resonance (EPR) spectroscopy with a spin-trapping technique, we find that OH and carbon-centered radicals are formed from the aqueous reactions of ISOPOOH with both iron(II) and iron(III) at room temperature. Kinetic modelling suggests that ISOPOOH can react with iron(II) via Fenton-like reactions leading to OH formation. Iron(III) is also found to react with ISOPOOH in a similar manner to generate OH radicals. In addition, the effects of metal-organic complexing on OH production were examined: oxalic acid largely affects the OH generated by ISOPOOH and iron reactions, likely due to oxalic acid forming a complex with iron. These findings contribute to our understanding and quantification of the role of organics and metals in ROS generation through atmospheric aqueous-phase chemistry.

5AC.2

Unambiguous Elucidation of the Structure and Formation Mechanism of Dimer Esters in Monoterpene Secondary Organic Aerosol. CHRISTOPHER KENSETH, Yuanlong Huang, Nicholas Hafeman, Nathan Dalleska, Brian Stoltz, John Seinfeld, *California Institute of Technology*

High-molecular-weight, low-volatility dimeric 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. In particular, covalent dimer esters have been routinely detected as major products in monoterpene SOA. Particle-phase reactions of closed-shell monomers [e.g., esterification and peroxyhemiacetal/diacyl peroxide decomposition] and gas-phase reactions involving early-stage oxidation products and/or reactive intermediates [e.g., stabilized Criegee intermediates (SCIs), carboxylic acids, and organic peroxy radicals (RO₂)] have been advanced as possible dimer ester formation pathways. However, the exact structures of the dimer esters, and thus the mechanisms underlying their production, remain unresolved, due in large part to the chemical complexity of the SOA matrix and, in turn, the speculative nature of structural assignments inferred solely from accurate mass and fragmentation data. Here, informed by detailed chromatographic and mass spectrometric (MS and MS/MS) analysis, coupled with ¹³C isotopic labeling, H/D exchange, and OH/SCI scavenging, we explicitly determine, for the first time to our knowledge, the molecular structures and abundances of select dimer esters in SOA derived from ozonolysis of α- and β-pinene through synthesis of authentic standards. Constrained by their molecular structures, the reactive intermediates and mechanism of dimer ester formation are unambiguously elucidated from a series of targeted SOA formation experiments. Identification of the chemistry underlying dimer ester production provides a missing link tying the atmospheric degradation of monoterpenes to the observed formation of low-volatility dimeric compounds capable of driving atmospheric particle formation and growth.

5AC.3

Kinetics and Equilibria for the Multiphase Formation of Hemiacetals and Peroxyhemiacetals. JULIA BAKKER-ARKEMA, Megan Claflin, Paul Ziemann, *University of Colorado*

Volatile organic compounds (VOCs) are emitted into the atmosphere and subsequently oxidized to form a variety of products containing carbonyl, carboxyl, hydroxyl, and hydroperoxy functional groups, many of which can partition into the particle phase to form secondary organic aerosol (SOA). Studies suggest that these products have the potential to undergo heterogeneous and multiphase reactions, and that these processes can influence the formation, composition, and physical-chemical properties of the aerosol phase. Due to the effects of organic aerosols on climate, air quality, and human health, many explicit chemical mechanisms have been developed to model the gas-phase oxidation of VOCs to form SOA in laboratory studies and in the atmosphere. However, these models largely fail to include the subsequent heterogeneous and multiphase chemistry that can occur within and on the surface of aerosol particles because there is limited experimental data providing the necessary kinetics, equilibria, and ambient concentrations of reactants and catalysts to properly model these reactions. In this work, we investigated two multiphase systems: the reactions of alcohols and carbonyls to generate hemiacetals, and the reactions of hydroperoxides and carbonyls to generate peroxyhemiacetals. Alcohol and hydroperoxide precursors were synthesized in the laboratory with a terminal nitrate group to provide a chromophore. Precursors were subsequently reacted with various carbonyl sources including ketones, aldehydes, and SOA generated in the laboratory from the ozonolysis of alpha-pinene with and without the presence of a catalyst. Reaction mixtures were analyzed by reversed-phase liquid chromatography with UV-Vis detection monitoring at 210 nm, where the terminal nitrate group demonstrates a strong absorbance. Products were collected and identified using electrospray ionization time-of-flight mass spectrometry (ESI-TOFMS). Forward and reverse rate constants and equilibrium constants were determined for each reaction. Together, these results improve our understanding of the heterogeneous and multiphase chemistry that can occur in SOA, and going forward will allow chemical models to more accurately capture SOA formation and composition.

5AC.4

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, Manjula Canagaratna, Jordan Krechmer, Rebecca Craig, Zhenfa Zhang, Avram Gold, John Jayne, Douglas Worsnop, Timothy Onasch, Cassandra Gaston, Joel A. Thornton, William Vizuete, Andrew Ault, Jason Surratt, *Univ. of North Carolina, Chapel Hill/Aerodyne Research, Inc.*

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. This laboratory study systematically examined the reactive uptake probability of isoprene-derived epoxydiols (γ_{IEPOX}) onto acidic ammonium sulfate particles with selected types of anthropogenic 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 was coated onto the acidic sulfate particles by using the potential aerosol mass (PAM) oxidation flow reactor, confirmed via atomic force microscopy (AFM) and scanning electron microscopy (SEM). Measured γ_{IEPOX} was parameterized as a function of SOA coating type, coating thickness, oxidation state, and RH. Results show that certain pre-existing anthropogenic SOA coatings significantly reduced the γ_{IEPOX} when compared with the γ_{IEPOX} for biogenic SOA coatings, in some cases by nearly an order of magnitude for the same coating thickness.

Particle composition was analyzed by both online and offline analytical techniques, including an aerosol chemical speciation monitor (ACSM) and ion mobility spectrometry-mass spectrometry (IMS-MS). A multivariant model combining the measured oxidation state and chemical compositions of the aerosols was constructed to predict the viscosity of SOA as a function of chemical compositions and RH. A box model with ambient measurements from the 2013 SOAS campaign was used to assess the effects of pre-existing organic coatings on IEPOX-derived SOA formation. Our results suggest that the chemical composition and RH jointly influence the phase state of SOA coating and subsequent multiphase chemical processes. The model developed during this study should be applicable to other multiphase chemical systems in regional- and global-scale models to better predict the impact of SOA on climate, human health, and visibility.

5AC.5

Modification of Aerosol Phase, Acidity, and Structure by Heterogeneous and Multiphase Chemistry. ANDREW AULT, Ziyang Lei, Nicole Olson, Yuzhi Chen, Yue Zhang, Andrew Lambe, Jason Surratt, *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, aerosol phase has been shown to range from to solid to semi-solid to liquid for ambient particles, Morphology (e.g. core-shell) of SOA with inorganic components (e.g. ammonium sulfate) 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. The changing water content of aerosols can impact acidity and reactive uptake of molecules such as isoprene epoxydiols (IEPOX). However, direct evidence of the impact of non-liquid phases and phase separation on heterogeneous uptake and continuing chemistry in aerosols is far more limited. Herein, we use atomic force microscopy (AFM) with phase images and photothermal infrared spectroscopy (AFM-PTIR), electron microscopy, and Raman microspectroscopy to probe phase, structure, and acidity of mixed SOA and ammonium sulfate particles in controlled laboratory studies (flow tube and chamber) and field measurements. Decreased uptake of IEPOX and conversion of inorganic to organic sulfate lead to important modifications of aerosol physicochemical properties and has large implications for aerosol impacts on air quality and climate.

5AC.6

Kinetics and Products of Multiphase Ozonolysis of Unsaturated Lipids. ZILIN ZHOU, Shouming Zhou, Jonathan Abbatt, *University of Toronto, Canada*

The heterogeneous ozonolysis reactions of multiple unsaturated lipids present in atmospheric aerosol and on household or human surfaces were studied. By using a new high-performance liquid chromatography/electrospray ionization mass spectrometry (LC-ESI-MS) method, the rapid decay of triolein (an unsaturated triglyceride in cooking oil arising from glycerol and oleic acid) in a thin surface film was observed. The reactive uptake coefficients (γ) were determined to be between $(4.2 \pm 0.8) \times 10^{-6}$ to $(1.5 \pm 0.3) \times 10^{-5}$ for films with average thicknesses between 4 and 40 nm. Stable secondary ozonides were observed to be the major condensed-phase products, along with a series of oxygenated compounds (acids and aldehydes) whose abundance exhibited a strong dependence on relative humidity (RH). Due to the unavailability of pure high-molecular weight secondary ozonides as internal standards, an ^1H NMR method was developed for the quantification of ozonolysis products, which involved the use of methyl sulfone as a universal reference. Results indicate that, under dry air, 65-80% of the ozonolysis products in triolein and methyl oleate are secondary ozonides that accumulate on the surface, whereas the remaining 20-35% of the reaction presumably yields volatile products (e.g. 1-nonanal) that are released into the air. Elevated relative humidity significantly suppresses the formation of ozonides in both lipids, making gas-phase products more favorable. In contrast, the yield of secondary ozonides and volatile products from ozonated oleic acid were $(16 \pm 2)\%$ and $(44 \pm 5)\%$ respectively, along with an insignificant dependence on relative humidity. The formation of high-molecular weight hydroperoxides were also observed. The environmental implications of this chemistry will be discussed from the perspectives of oxidative aging of lipids in atmospheric aerosol and volatile species affecting indoor air quality.

5AC.7

Laboratory Studies of ClNO₂ Production from N₂O₅ Uptake on Saline Playa Dusts. CASSANDRA GASTON, Dhruv Mitroo, Thomas Gill, Savannah Haas, Kerri Pratt, Haley Royer, *University of Miami*

Nitryl chloride (ClNO₂), formed when dinitrogen pentoxide (N₂O₅) reacts with chloride-containing aerosol, photolyzes to produce chlorine radicals that facilitate the formation of tropospheric ozone. ClNO₂ has been measured in continental areas; however, the sources of particulate chloride required to form ClNO₂ in inland regions remain unclear. Dust emitted from saline playas (e.g., dried lakebeds) contains salts that can potentially form ClNO₂ in inland regions. Here, we present the first laboratory measurements demonstrating the production of ClNO₂ from playa dusts. N₂O₅ reactive uptake coefficients ($\gamma_{N_2O_5}$) ranged from $\sim 10^{-3}$ to 10^{-1} and ClNO₂ yields (ϕ_{ClNO_2}) on playa dusts were >50% for all playas tested except one. In general, as the soluble ion fraction of playa dusts increases, $\gamma_{N_2O_5}$ decreases and ϕ_{ClNO_2} increases. We attribute this finding to a transition from aerosol surfaces dominated by silicates that react efficiently with N₂O₅ and produce little ClNO₂ to aerosols that behave like deliquesced chloride-containing salts that generate high yields of ClNO₂. Molecular bromine (Br₂) and nitryl bromide (BrNO₂) were also detected, highlighting that playas facilitate the heterogeneous production of brominated compounds. Our results suggest that parameterizations and models should be updated to include playas as an inland source of aerosol chloride capable of efficiently generating ClNO₂.

5AE.1

Modeling Ambient Air Quality at Exposure Relevant Scales using the Community Earth System Model. FORREST LACEY, Rebecca Schwantes, Simone Tilmes, Colin Zarzycki, Louisa Emmons, Marsh Daniel, Walters Stacy, Francis Vitt, Gabriele Pfister, Peter Lauritzen, Alma Hodzic, *National Center for Atmospheric Research*

Modeling ambient air pollution is difficult due to the complex interactions between the atmosphere and other Earth systems. This is especially challenging when considering how changes in anthropogenic activity and subsequently climate will shift the formation and fate of aerosols throughout the next century. Commonly, chemical transport models (CTMs) are used to estimate human exposure to trace pollutants, such as fine particulate matter (PM_{2.5}) and ozone, although these methods do not include many of the climate and Earth system feedbacks that are necessary to accurately predict future changes in ambient air quality. Here we will present comparisons of observed aerosol concentrations over the United States during 2013 with modeled concentrations using a newly developed fully coupled global state-of-the-science Earth system model with variable resolution ("CAM-chem-SE-RR"). This model is a configuration of version 2 of the Community Earth System Model (CESM2) that allows us to isolate the benefits of increasing model resolution, emission spatial and temporal resolution, and model chemical complexity. These results are then combined with exposure response functions to estimate the human health impacts from ambient air pollution for 2013 including sector and region-specific source attribution for these impacts. The conclusions from this analysis show that the combination of exposure-relevant resolution (~ 14 km over the contiguous U.S.), detailed atmospheric chemistry, and the inclusion of earth system feedbacks, all within a global model, allows for more accurate predictions of air quality than previous methods by considering the bi-directional interactions over local to global scales making this model a new and powerful tool for future air quality predictions.

5AE.2

Improving Daily Surface Particulate Matter Estimates during Extreme Fire Events using a Novel NASA Satellite Plume Injection Height Algorithm. S. MARCELA LORÍA-SALAZAR, Jingting Huang, Jaehwa Lee, Andrew Sayer, Neil Lareau, Heather Holmes, Jens Redemann, *University of Oklahoma*

Climate change has increased the frequency of droughts in recent decades and consequently, the occurrence and severity of wildfires have amplified, especially in the western U.S. Wildfires are important to maintain the ecological equilibrium of the landscape but smoke emissions represent a global public health problem impacting vulnerable populations and the economy. Near extreme fire events, satellite characterization of thermal anomalies is desired because it can capture the horizontal extent of the smoke plume. However, air quality (AQ) models based on satellite retrievals have been challenged during fire periods because of the limitation in detecting small fires, large fires events which consequently produce pyrocumulus clouds, and the underestimation of aerosol loading due to very rigorous fire filters in the satellite algorithm. Satellite fire radiative power provides daily burning areas but the information is very localized and not designed to estimate the transport of the plumes to other areas away from the source. With these limitations in mind, this research presents an AQ fire ratio (AQFR) which can distinguish the vertical distribution of aerosols as the smoke plumes were transported downwind, and if the smoke was able to reach the surface or penetrate the free troposphere using a combination of numerical weather prediction model outputs and a novel plume injection height algorithm from NASA ASHE VIIRS during the fire seasons of 2013-2014 in the U.S. Preliminary results in the western U.S. using the MODIS version of the ASHE algorithm have shown that differences in meteorological conditions affecting the planetary boundary layer (PBL) physics during the day can impact the percentage of confinement of the fire plumes within the PBL. The use of this novel AQFR will aid in quantifying the health effects and can improve AQ forecasting models due to wildfire smoke.

5AE.3

Environmental Justice and Fine Particulate Matter Exposure in California. SARAH CHAMBLISS, David Paoletta, Christopher Tessum, Joshua Apte, Julian Marshall, *University of Texas at Austin*

Studies investigating environmental justice (EJ) issues in air pollution have found that non-white communities experience higher exposure to air toxics, diesel particulate matter, and other PM_{2.5} constituents. With recent advances in reduced-complexity air quality models, researchers have expanded EJ analyses to include all major sources of anthropogenic air pollution and consider effects throughout the United States. In this study, we quantify the exposure disparities by race and socioeconomic status that result from anthropogenic emissions within the state of California and surrounding areas, with a view to identify control strategies with substantial EJ benefits. We use a version of the InMAP Source-Receptor Matrix centered around the state of California to examine the contribution of 60 major categories of primary PM_{2.5} and precursor emissions to exposure across a range of demographic groups. We find that compared to a population-weighted average concentration of 6.8 µg/m³, the white population average concentration is lower by 18%, while Hispanic, Asian, and black populations experience 17%, 6%, and 15% higher concentrations. Industrial emissions sources contribute most to this disparity, followed by on-road mobile sources, with the total magnitude and importance of different subcategories varying by race. Primary PM_{2.5} contributes more (61-63%) to exposure disparity among black and Asian populations, while the increased exposure among Hispanics is less strongly influenced by secondary PM_{2.5} (38%). When stratifying results by income, we see that exposure varies by income for white and Asian populations, but there is no relationship between exposure and income for Hispanic and black populations. These nuanced results reveal a number of possible strategies for reducing overall PM_{2.5} exposure and reducing exposure inequity in California and its surroundings.

5AE.4

Near-Source Spatial Extents and Socio-Economic Disparity in Urban Air Pollution Exposure. RISHABH SHAH, Ellis Shipley Robinson, Peishi Gu, Joshua Apte, Allen Robinson, Albert A. Presto, *Carnegie Mellon University*

Primary carbonaceous aerosols (PCA) e.g., cooking organic aerosol (COA), hydrocarbon-like OA (HOA), and black carbon contribute ~ 50% mass of urban fine particulate matter, and have large spatial variabilities, exerting adverse health effects. Different intra-urban neighborhoods have different socio-economic features, and thus neighborhood-scale air quality impacts of restaurants and highways may result in certain socio-economic groups being exposed to higher pollutant concentrations. Our objective is to: a) characterize spatial extents to which urban sources influence PCA concentrations, and b) examine the socio-economic disparities in PCA exposure.

We use high- spatial-resolution data from mobile aerosol mass spectrometry measurements in Oakland CA and Pittsburgh PA. By binning our measurements into “distance-from-source” bins, and using a simple power law model, we are able to quantify distance-decay patterns of PCA e.g., decay of COA concentrations with distance from restaurants. We calculate characteristic length-scales of influence (d_f) of restaurants in Oakland and Pittsburgh to be ~ 150 and 450 m, respectively. The larger d_f in Pittsburgh is explained by its larger density of restaurants. Similarly, we calculate d_f for highways.

Socio-economic analyses of census tract data reveals minor disparities in exposure to highway emissions, but large disparities in exposure to COA concentrations near restaurants. In areas strongly influenced by cooking emissions (within d_f meters of restaurants), poverty is 1.2× higher, and household income is 0.7× lower relative to uninfluenced areas, suggesting that with poor people are far more likely to be exposed to near-source COA enhancements than prosperous people. Further, we find large racial-ethnic disparities in COA exposure: White (-1%), Black (2%), Hispanic (8%), Asian (12%), Other (5%). While we will perform additional analyses, preliminary results indicate that non-White population in both Oakland and Pittsburgh is exposed to higher-than-average COA concentrations, while White population is exposed to equal or below average COA levels.

5AE.5

Spatial Correlation of Ultrafine Particle Number and PM2.5 Mass Concentrations: Implications for Health Assessment. PROVAT SAHA, Shayak Sengupta, Joshua Apte, Peter Adams, Allen Robinson, Albert Presto, *Carnegie Mellon University*

There are growing concerns that adverse health effects of ambient ultrafine particles (UFP, diameter < 100 nm) may differ from those of currently regulated fine particulate matter (PM2.5) mass concentrations. However, the epidemiological evidence of whether UFP have chronic health effects independent of PM2.5 mass remains inconclusive or insufficient. The correlation between PM2.5 mass and UFP concentrations influences the ability of epidemiological studies to differentiate their health effects. To assess the spatial correlation of UFP and PM2.5 mass, we integrate insights from temporally and spatially rich measurements, land-use regression (LUR), and a high-spatial-resolution chemical transport model (CTM). We conducted 3-6 weeks of continuous measurements of particle number concentrations (PNC; a proxy for UFP) at 32 sites, and year-long continuous measurements of PM2.5 at 50 sites in Pittsburgh, Pennsylvania covering a wide range of urban land-use attributes. While PNC are more spatially heterogeneous than PM2.5 mass, they are spatially moderately correlated in our data set ($R^2 \sim 0.3$, $N = 30$ sites). LUR models derived from these measurements explains about 80% of the spatial variability in PNC using traffic, commercial land use, and population density as predictors; PM2.5 LUR model explains about 60% variability with commercial and residential land use, population and point emission sources. The LUR-predicted PNC and PM2.5 concentration surfaces for the city of Pittsburgh are moderately correlated ($R^2 \sim 0.4$). High-spatial-resolution (1km) CTM simulations show that PNC and PM2.5 are highly correlated ($R^2 \sim 0.8$) in intra-urban scale. Our simulations and measurements suggest that the intra-urban spatial differences in PNC and PM2.5 mass concentrations are driven by primary emissions. The implication is that the PNC-PM2.5 mass correlations will make it difficult to isolate the independent health effects of UFP in epidemiological studies at the intra-urban scale.

5AE.6

Land Use Regression Models of Traffic-Related Semi-Volatile Organic Pollutants in an Urban Area with Elevated Prevalence of Pediatric Asthma. Sarah Esenther, Elizabeth Lin, Laura Minet, Marianne Hatzopoulou, KRYSTAL GODRI POLLITT, *Yale University*

The spatial variance of select traffic-related air pollutants (PM_{2.5} mass, black carbon and nitrogen dioxide (NO₂)) has been evaluated using land use regression (LUR) methods in numerous geographic regions. Spatial models of PM composition and specifically the organic fraction is lacking. One challenge in building LUR models is the collection of simultaneous samplers at multiple sites to measure airborne organic pollutants. To facilitate assessment of this organic fraction we developed a low-cost air pollutant sampler. The device passively absorbs semi-volatile organic compounds (SVOCs) into a polydimethylsiloxane sorbent material which were analysed off-line by thermal desorption high resolution gas chromatography mass spectrometry. NO₂ is also measured by the sampler using an Ogawa pad. The objective of this study was to demonstrate the utility of this low-cost sampler for measuring SVOCs at multiple sites and use these measurements to build LUR models for individual organic components. We evaluated Springfield, Massachusetts given the elevated prevalence of pediatric asthma (19%) compared to the state average (11%) coupled with the recognised sensitivity of asthmatic children to traffic-related air pollutants. It was of interest to use SVOC LUR models to identify regions with increased tailpipe and non-tailpipe derived pollutant levels. Forty samplers were deployed across Springfield (~185 km²) at urban and suburban sites for five consecutive weekdays in June 2018. A five-day time-integrated average concentration of SVOCs were measured at each site. Six compounds had detectable concentrations at 20 or more of the sample locations. LUR models were built for these SVOCs as well as NO₂ using built environment and land use characteristics. These exposure surfaces will be compared with personal exposure measurements from a cohort of asthmatic children in Springfield and further serve as a valuable resource for the analysis health outcomes and risk assessment.

5AE.7

Children's Particulate Matter Exposures Characterization as Part of the New Hampshire Birth Cohort Study. Michelle McCombs, JONATHAN THORNBURG, Seung-Hyun Cho, Nalyn Siripanichgon, Erin Butler, Margaret Karagas, *RTI International*

The New Hampshire Birth Cohort Study (NHBCS) is an ongoing, prospective study of rural pregnant women and their children, and a pediatric cohort for the NIH-funded Environmental influences on Child Health Outcomes (ECHO) program. The primary aim of the NHBCS is to investigate the effects of environmental exposures, including use of wood stoves, on fetal growth and childhood development.

A subset of children 3 to 5 years old, nearly 25% of whom live in a home with a wood stove as the primary heating source, participated in a personal monitoring study of PM_{2.5} exposures. This study is the first to report personal PM_{2.5} exposure using a wearable sensor on children younger than 5 years, not proximity measurements. Three days' worth of physical activity and personal air monitoring were collected using the MicroPEM™ for PM_{2.5}.

To date, 272 children have been enrolled in the study to wear the MicroPEM for 72 hours. Exposure data were collected successfully from 244 participants who had more than 48 hours of participation. Participants wore the MicroPEM an average of 70% of their time awake. Across all participants, real-time filter corrected nephelometer PM_{2.5} concentrations showed a mean of 23.1 µg/m³ (standard deviation, SD = 136). Each filter was analyzed for speciation of environmental tobacco smoke (ETS), black carbon (BC), and brown carbon (Br). Average values were 4.2 µg/m³ ETS (SD = 6.1), 0.5 µg/m³ BC (SD = 3.1), and 0.9 µg/m³ BrC (SD = 1.0). Personal PM_{2.5} data showed higher values for winter-spring months versus other months of the year.

Personal sensors can be worn by young children to measure their air pollution exposure and advance environmental epidemiological research. The data shows seasonal differences in PM_{2.5} as well as higher levels of ETS exposure over BC and BrC.

5BC.1

New Insights into the Health and Climate Impacts of Boreal Wildfires. SARAH STYLER, Ming Lyu, Iris Chan, Nianci Zhang, Matthew S Ross, Cora J. Young, Daniel K Thompson, *University of Alberta*

Over the past three summers, the Fort McMurray wildfire and wildfires across British Columbia released significant amounts of smoke and ash into the atmosphere, which resulted in substantial air quality reductions across western Canada. Wildfire ash contains toxic polycyclic aromatic hydrocarbons (PAH), which are known to undergo a variety of transformations on environmental surfaces. Here, we investigate the light- and ozone-mediated loss of PAH at the surface of ash samples obtained from the Fort McMurray wildfire. Since the toxicity of PAH ozonation products is often greater than that of the parent compounds, these experiments provide insight into the long-term health impacts of fires at the wildland–urban interface.

A major contributor to the particulate matter component of wildfire emissions is brown carbon (BrC), a class of light-absorbing organic carbon that can affect climate by altering Earth's radiative balance. Although many studies have investigated the composition and properties of BrC, comparatively few studies have focused specifically on characterizing BrC produced from boreal wildfires. Here, we use size-exclusion chromatography with diode-array UV-Vis absorption detection to study the light-absorbing properties of particulate matter produced via combustion of boreal peat samples obtained in northern Alberta. We find that the composition and optical properties of fresh boreal peat BrC differ substantially from aged ambient wildfire BrC and also vary substantially with peat moisture content and sampling depth. Together, these results highlight the importance of performing experiments under realistic combustion conditions, and help to bridge lab studies of fresh BrC with field measurements of aged BrC.

5BC.2

Regional Transport of Biomass Burning Aerosols in Northern South America and its Contribution to POA and SOA in Colombian Cities. KAREN BALLESTEROS, Maria Alejandra Rincón, Juan Manuel Rincón, Amy P. Sullivan, Ricardo Morales Betancourt, *Universidad de los Andes*

Fine particulate matter (PM_{2.5}) concentration in Colombian cities often exceeds local limits, and customarily exceeds WHO guideline concentrations. Because of the high degree of urbanization in the country, the focus in air quality studies has been on the contributions of local sources, mainly mobile and industrial, to the urban environment. Therefore regional sources such as open biomass burning, and long-range transport of mineral dust have often been neglected. Recent works, however, have compiled evidence suggesting a strong correlation between the number of fires in Northern South America (NSA) and deteriorated ambient air quality in some Colombian cities. These results indicate a potentially important seasonal contribution of regional sources to high air pollution levels in densely populated areas. In this work, we assess the contribution of open biomass burning events to particulate matter (PM) in urban environment using an atmospheric regional chemical transport model (WRF-Chem). The model was configured in a large parent domain of 3200 km (121x121x40) encompassing NSA, and two higher-resolution nested domains. The horizontal resolution of each domain is 27x27 km, 9x9 km, and 3x3 km respectively. Anthropogenic emissions for the domain were extracted from EDGAR v4.3.1, and were merged with a local emission inventory for the city of Bogotá. Biogenic emissions from MEGAN were also included in the simulations. The contribution from biomass burning to PM in Colombian cities was evaluated through a sensitivity analysis in which two scenarios, FIRE and NOFIRE, were constructed. In these scenarios fire emissions from the FINN inventory are turned on and off respectively. Model performance was evaluated by comparing simulation results against in-situ observations from air quality networks, remote sensing data, and speciated PM_{2.5} from measurements campaigns. Results indicate an increment on PM_{2.5} concentration over Bogotá when biomass burning emissions are included in the simulation. This increment is shown to be mainly driven by Secondary Organic Aerosols (SOA) suggesting that POA from biomass burning emissions is not a significant contributor to fine particulate in Bogotá. This is likely due to the high gas-phase SOA precursors emitted from open biomass burning and the typical three days of aging endured by the fresh biomass burning plumes before reaching the city.

5BC.3

Airborne Characterization of Wildfire Influence on Local Air Quality in California. Nilima Sarwar, Walt Williams, Armin Sorooshian, Hafliði Jonsson, Richard Flagan, John Seinfeld, ANDREW METCALF, *Clemson University*

In many regions, wildfires contribute significantly to airborne particulate matter. Many factors influence the degree to which these fires affect local air quality, including fire size, fuel type, stage of the fire, meteorology, and co-located pollution sources. In early summer of 2018, several wildfires were encountered in Northern California which influenced air quality in the San Francisco Bay and Sacramento Valley areas. These areas were sampled by the Naval Postgraduate School's Twin Otter aircraft, which was instrumented with a payload focused on aerosol characterization. The payload included multiple aerosol size and optical property measurements, aerosol chemical composition by an aerosol mass spectrometer, and black carbon (BC) aerosol by a Single Particle Soot Photometer (SP2).

In this talk, these aerosol measurements are used to assess the influence of two wildfires on the background air in the region. One fire, the County Fire, was a ~90,000 acre fire and was sampled several days after it was ignited and well before it was fully contained. The second fire, the Pawnee Fire, was much smaller, at ~15,000 acres, and was sampled on the last day of its active burning. Noticeable differences in the vertical extent of each plume and the ease with which each plume was identified were seen in the BC and total aerosol number and mass concentrations. Particle size distributions are analyzed to separate the urban from biomass burning plumes. Finally, aerosol composition measurements of the biomass plumes align well with expected values from lab studies of combustion with similar fuels. These two wildfire case studies provide contrasting examples of the influence wildfires can have on local air quality.

5BC.4

Chemical and Physical Properties of Smoke Plumes in the Western and Southeastern US Using Hazard Mapping System (HMS) and AERONET/IMPROVE Data. QIJING BIAN, Bonne Ford, Jeffrey R. Pierce, Sonia Kreidenweis, *Colorado State University*

Biomass burning is a major source of summertime PM_{2.5} in the US. Emissions degrade air quality and are associated with negative effects on human health. According to data compiled in the National Emissions Inventory, wildfires dominate biomass burning emissions in the west while prescribed fires dominate emissions in the southeast. The different fire sizes, fuel types, and emission factors from wildfires and prescribed fires may produce emitted smoke particles with different properties, e.g. particle size, chemical composition and optical properties. We used data from the Hazard Mapping System (HMS) to track smoke plumes for 10 years from 2008 to 2017. Combining these geospatial data with AERONET data, we define "smoke days" at a particular site as those days when the smoke polygon from HMS included the coordinates of that site and only compile data for April through September, for both smoke days and non-smoke days. For the IMPROVE network, we further apply a threshold of PM_{2.5} larger than mean + standard deviation in the target year, so we can filter out the cases where the smoke is not at the surface. We derive the composition of smoke PM_{2.5} using the difference between smoky and non-smoky days. We find that elemental carbon (EC) fraction of smoke in the southeast is about half of the EC fraction in the west, consistent with more smoldering prescribed fires in the southeast. For AERONET data, inverted size distributions show that western smoke had smaller-diameter fine particles than southeastern smoke, but more coarse particles, perhaps associated with lofting of dust by western wildfires. We found that the single scattering albedo (SSA) of smoke varied from 0.937-0.946 in the west to 0.962 in the southeast, consistent with the differences in EC fraction and fire types. Higher relative humidity in the southeast may also contribute to the higher smoke SSA relative to the west. Hence, differences in fire types and conditions between the west and southeast may contribute to differences in smoke composition and optical properties.

5BC.5 (INVITED)

Smoke Forecasting for Wildfires – Interdisciplinary Tools and Operational Applications. SUSAN O'NEILL, Narasimhan Larkin, Yufei Zou, Sean Raffuse, Peter Lahm, Mark Fitch, *USDA Forest Service*

The science and skill of wildfire smoke forecasting is built upon an interdisciplinary array of tools, data, models and expertise, ranging from on the ground fuels and fire behavior measurements, to what the satellites see from space. Wildfire smoke, as the most visible part of a wildfire especially to the general public, can have the furthest reaching consequences in terms of health, visibility and socio-economics. Health impacts can include cardiorespiratory symptoms and even mortality and the costs associated with these health impacts can exceed fire-fighting costs. Furthermore, as wildfire seasons get longer and more intense and smoke impacts not only rural communities but large metropolitan areas, the need for information about smoke is mounting. The public wants to know; How do I protect myself? When is the smoke going to clear? Is the air safe enough for my kids to play outside? Do we cancel the Ironman? Answers to these questions rely on science that informs tactical decisions and impacts to public health. This talk will highlight the array of tools and information useful for smoke forecasting such as smoke modeling systems, smoke monitoring networks and remotely-sensed data. The process of merging these disciplines and data, we call putting on our smoke glasses. The emphasis will be on the science under-lying these systems across disciplines and the variability and uncertainty associated with the data and information. We will also talk about the Wildland Fire Air Quality Response Program (WFAQRP), which works with the wildfire incident command structure providing smoke monitoring, smoke modeling and consistent messaging about smoke to health and air quality agencies and ultimately the public. As an example of how these many tools and information are used, we will profile the smoke forecasting work of Air Resource Advisors deployed as part of the WFAQRP.

5BC.6

Next Generation Wildfires: Firestorms at the Urban-Wildland Interface. KEITH BEIN, Irva Hertz-Picciotto, Anthony S. Wexler, *University of California, Davis*

Due to climate change, wildfires are increasing in size, frequency, duration and severity accompanied by longer fire seasons and larger geographical areas of susceptibility. Concomitantly, human development continues to expand and the boundary between remote wildlands and densely populated regions decreases, making large populations of people vulnerable to large scale wildfires that used to be remote, isolated occurrences. A striking example of this was the Northern California Firestorm in October 2017 that devastated several neighborhoods and business districts throughout Napa and Sonoma Counties, perhaps most notably Coffee Park in Santa Rosa. This was an unprecedented event where a substantial fraction of combustion involved construction materials, consumer products, infrastructure, common household items and various other substances rather than biomass. Although wildfires have been studied for decades and there is a substantial body of literature characterizing biomass combustion emissions, there is a huge knowledge gap in the composition, and subsequent toxicity, of these emissions when wildfires cross boundaries into urban and residential areas. A Rapid Response Mobile Research Unit has been designed and built to address this knowledge gap. Preliminary results from deployment of this unit in the 2017 and 2018 Northern California wildfires will be presented.

5IA.1

Response of Eight Low-Cost Particle Sensors and Consumer Device to Typical Indoor Emission Events. YANGYANG ZOU, Matthew Young, Andrew May, Jordan Clark, *The Ohio State University*

Low-cost particle sensors may have the potential to transform smart building systems by providing continuous or semi-continuous measurements of indoor air quality. However, due to the rapid growth in the marketplace of available particle sensors, the practical use of some of the technologies is uncertain due to a lack of a rigorous evaluation of their performance. In this study, we evaluated a suite of these products, including three bare sensors (BS) and five integrated devices (ID; which contain one or more of these sensors and often some additional features such as wireless connectivity). Using a test home on The Ohio State University campus, we co-located these sensors with reference instruments for nearly three months. Over the duration, we generated particles inside the home using several common sources of indoor particles, including burning incense, candles, and toast; using deodorizing and disinfecting sprays; operating a humidifier; and opening the windows.

All of the BS and ID were able to respond to the different sources, but in general, the magnitude of the responses varied for the different sensors. For example, the ratio of the time-integrated mass concentration from the sensors to the reference instruments varied from close to zero to greater than three. Moreover, there were some source-specific response effects that appear to be related to the size distributions of the particle sources; for some sources, the sensors' response was linear with a slope and coefficient of determination (R^2) close to unity, but in other cases, the slopes and R^2 values were much poorer. Performance was generally best when source of particles was an open window, which is consistent with many field evaluation studies of these low-cost particle sensors.

5IA.2

Ultrafine Particle Dynamics in a Net-Zero Energy House: Application of a Building Energy Management System for Evaluating Source and Loss Processes. JINGLIN JIANG, Brandon E. Boor, *Purdue University*

Research on net-zero energy buildings (NZEBS) has been largely centered around improving building energy performance, while little attention has been given to indoor air quality and aerosols. An important step towards improving indoor air quality in NZEBs is understanding how occupants, their activities, and building systems affect the emissions and fate of ultrafine particles (UFPs). New developments in building energy management systems (BEMS) and smart thermostats offer a unique opportunity to track occupant activity patterns and the operational status of residential HVAC systems. The objective of this study is to investigate how a BEMS can be used to characterize time-variant UFP source and loss processes in an occupied residential NZEB.

A one-month field campaign was conducted at the Purdue ReNEWW (Retrofitting Net-zero Energy, Water, and Waste) House. Three adult residents occupied the house throughout the campaign. A scanning mobility particle sizer and optical particle sizer were used to measure indoor aerosol concentrations and size distributions from 10 to 10,000 nm. AC current sensors monitored electricity consumption of electrical kitchen appliances (cooktop, oven, toaster, microwave), the air handling unit (AHU), and the energy recovery ventilator (ERV). Two smart thermostats informed the fraction of supply air delivered to the basement and main floor of the house. BEMS-based data was integrated with the aerosol measurements and a material balance model to determine size-integrated UFP (10 to 100 nm) source and loss rates.

The ReNEWW House BEMS data identified hourly and weekly use-profiles and active emission periods of the four electrical kitchen appliances and the runtime of the HVAC system. The BEMS identified cooking activities as the dominant UFP source in the ReNEWW House, often elevating indoor UFP concentrations beyond $10,000 \text{ cm}^{-3}$. UFP concentrations were the greatest when using the oven, with a median value of $6,400 \text{ cm}^{-3}$. Kitchen appliance usage was most frequent between 10:00 and 14:00 and 18:00 and 21:00. Mean number size distributions for each appliance were determined during active emission periods and exhibited modal diameters between 20 and 50 nm. The HVAC system runtime exhibited a diel trend, thereby driving transient variations in HVAC-associated UFP source and loss processes. The AHU runtime peaked at around 10:00, reaching 74%, and was the lowest from 02:00 to 07:00, at around 36%. The ERV operated on a fixed schedule with a runtime of 36%. UFP source rates for the kitchen appliances inferred from the BEMS-aerosol data varied from 10^{11} h^{-1} to 10^{14} h^{-1} . Median UFP loss rates when the AHU/ERV were off and on were 1.4 h^{-1} and 3.7 h^{-1} , respectively.

5IA.3

Measurements of Fine and Ultrafine Particles Emitted by Marijuana Sources Indoors in a Residence. Wayne Ott, Kai-Chung Cheng, TONGKE ZHAO, Lance Wallace, Lynn M. Hildemann, *Stanford University*

Ten states in the U.S. have legalized recreational marijuana, but few studies have been done measuring exposure to secondhand marijuana smoke in everyday settings. Popular ways to smoke marijuana include a *glass pipe* containing cannabis buds, a pre-rolled *joint* similar to a cigarette or cigar, a water pipe or *bong*, a *vaping* pen that vaporizes cannabis oil from a commercial cartridge, and a *blunt*, which is a hollowed out cigar filled with marijuana. All these marijuana sources produce PM_{2.5}, which is also produced by conventional tobacco cigarettes and cigars and is of concern because of its possible health effects.

We conducted controlled experiments with a human smoker indoors in a 43 m³ residential bedroom using two TSI Piezobalances, two TSI AM510 SidePak monitors, and a pair of TSI Condensation Particle Counters. Unlike conventional cigarettes, marijuana is often smoked one puff at a time, with a time gap between puffs. Our initial results show indoor emissions from different methods of smoking marijuana ranged from 1.4 to 3.1 mg/puff, with a pre-rolled joint producing the largest emissions. Since marijuana joints come in many shapes and sizes, we compare a variety of different marijuana joints with conventional cigarettes. While a regular tobacco cigarette may produce less PM_{2.5} per puff than a marijuana joint, conventional cigarettes usually are smoked in a manner different from marijuana -- the puffs are repeated until the tobacco is used up, so a comparison of the two types of smoking should take this difference into account. We discuss the basic methodology used to calculate source strengths, emission rates, and decay rates in the room of a home, illustrating the methodology with experimental data. This is one of the first systematic measurement studies of the effect of marijuana use on indoor air quality.

5IA.4

Criegee Intermediate Driven Autooxidation of Lipid Aerosol Surfaces. MEIRONG ZENG, Nadja Heine, Kevin Wilson, *Lawrence Berkeley National Laboratory*

Lipids are the essential nutrients for humans and are important structural components in cell membranes. Lipid oxidation, which plays a central role in aging-related diseases and food systems, have long been thought to be a solely driven by the formation and decomposition of hydroperoxides, a process known as lipid autooxidation. Recently, we found evidences for an alternative mechanism involving the formation and subsequent chemistry of Criegee intermediates (CI) produced when unsaturated lipids are exposed to hydroxyl radicals (OH). A series of model compounds, with different numbers and substituents of C=C bonds: squalene (Sqe), 9-tricosene, oleic acid, linoleic acid, and arachidonic acid, were investigated in a continuous flow stirred tank reactor. For Sqe, aldehydes and secondary ozonides (SOZs) are detected as major products using a vacuum ultraviolet aerosol mass spectrometer. The detection of SOZs, generally observed only in ozonolysis experiments, provides a distinctive signature of Criegee intermediate reaction pathways. To further confirm this, 2-decyl-1-tetradecanol, a Criegee scavenger, was added to the lipids + OH experiments. The detection of α -alkoxylalkyl hydroperoxides, produced from the Criegee and scavenger reactions, further confirms the importance of CI in the heterogeneous lipids and OH oxidation. Effective uptake coefficients of Sqe increase from 1 to 70 upon decreasing [OH] from 2×10^8 to 6×10^5 molecules/cm³, which clearly indicate the importance role that CI play in the autooxidation chemistry of Sqe under typical indoor OH concentrations. A kinetic model, built with Criegees based pathways, can reasonably reproduce these experimental results. This work provides potential link typing present Criegee-driven autooxidation mechanism to the OH involved dehydration of human and food lipids, as well as evolution of atmospheric unsaturated aerosols.

5IA.5

Indoor Black and Brown Carbon from Cooking Activities and Outdoor Penetration. SUMIT SANKHYAN, Sameer Patel, Delphine K. Farmer, Marina Vance, *University of Colorado Boulder*

For energy efficiency, buildings nowadays are being made more airtight with lower air exchange rates resulting in decreased penetration of air pollutants of outdoor origin. However, the same building characteristics might result in higher and prolonged exposure of air pollutants of indoor origin. Particulate matter (PM) emissions from cooking activities are a major contributor to indoor air pollution. Optically absorbing carbonaceous aerosols mainly black carbon (BC) and brown carbon (BrC) are an important constituent of PM emissions whose health effects are closely associated with PM exposure.

The results presented here are from the HOMEChem field campaign conducted in a three-bedroom, two-bathroom manufactured test house maintained at a relatively constant air exchange rate. Two five-wavelength aethalometers measured real-time BC and BrC concentration indoors as well as outdoors. Indoor to outdoor ratios (I/O) of BC and BrC concentrations were calculated for periods of inactivity inside the house as well as during experiments including the preparation of different types of meals. An overall penetration factor for BC was also calculated to understand the role of building envelope on BC infiltration from outdoors. The power law fitting approach for aerosol light absorption was used to calculate the angstrom exponent (α) during various cooking events. The α value ranged from 1.09-3.48, with an increase in the value of α being attributed to non-BC emissions during periods of intense cooking activities. BC exposure was calculated for the kitchen microenvironment and to direct the attention to the role of cooking activities on indoor air quality in terms of BC emissions.

5IA.6

Impacts of Rooftop Vegetation on HVAC Filter Loadings and Indoor Air Quality. PRADEEP RAMASUBRAMANIAN, Irvan Luhung, Elliott Gall, *Portland State University*

Resuspension of biotic particles from green roof substrate or vegetation on building rooftops may contribute to additional biomass loading on HVAC filters, influencing the quality of ventilation air. For example, volatile organic compounds (VOCs) emitted from biotic material trapped on the filter can subsequently react with ozone or other oxidants entering the ventilation system, resulting in secondary organic aerosol (SOA) or reaction products entering the indoor space. This study investigates the potential for green roofs to impact indoor air quality (IAQ), by investigating the microbiome, emissions, and chemistry occurring due to the particle loadings on HVAC filters near green roofs. HVAC filters were collected from two air handling units (AHUs) at a field site in Portland OR containing both green and white rooftop types. Experiments were conducted to characterize the microbial loading, VOC emissions and byproduct/SOA formation from the filters. The microbiome of the green roof filters (GRF) vs. white roof filters (WRF) were characterized by quantitative polymerase chain reaction (qPCR) and metagenomic sequencing on Illumina HiSeq platform. Primary VOC emissions were identified using proton transfer reaction – time of flight – mass spectrometry (PTR-TOF-MS), measuring the differences in the balance and type of volatile emissions due to loaded mass on GRF vs. WRF. Ozone was then injected upstream the filter, to measure ozone removal due to filter loading and a scanning mobility particle sizer (SMPS), measuring particles 10-420 nm, was placed after the filters to assess the potential for SOA formation due to oxidation processes on the filter. Preliminary measurements indicate differences in filter loadings that could potentially impact the quality of ventilation air.

5IA.7**Database for Aerosols on the International Space Station.**

MARIT MEYER, Meytar Sorek-Hamer, *NASA Glenn Research Center*

The microgravity environment affects the sizes and types of aerosols in the indoor living spaces of a spacecraft. Particle behavior is non-intuitive without gravitational settling, and astronauts must contend with airborne particles on the order of hundreds of micrometers and larger, in addition to the smallest sizes we are accustomed to on Earth. Aerosol sampling has taken place on the International Space Station (ISS) twice, with the archival samples returned to Earth, resulting in a large body of data from microscopy. Many of the collected particles have unusual morphologies and contain a large variety of metals. As this was the first opportunity to study particles on a long-duration space mission, the initial analysis approach with the results focused on understanding what is airborne, including some source apportionment. In order to make the data more useful to stakeholders within NASA, a database of analyzed particles was created. The search feature queries all analyzed particles by different particle characteristics, including material, diameter, shape characteristics, ISS location, etc. The output gives statistics on the different types of particles and show ISS locations where emission sources are significant. This information can be used to determine whether particle-producing materials or processes should be changed to reduce ISS aerosols. The first step in identifying whether particle sources should be mitigated is to identify ISS aerosols containing materials with known toxicity or health effects. Several case studies of undesirable ISS particle classes will be highlighted in this talk.

5IM.1**Intercomparison of an EESI-TOF with VOCUS-PTR for**

Quantitative Aerosol Analysis. DONGYU S. WANG, Chuan Ping Lee, Jordan Krechmer, Manjula Canagaratna, Francesca Majluf, Yandong Tong, Josef Dommen, Andre S.H. Prévôt, Imad El Haddad, David Bell, Jay G. Slowik, Urs Baltensperger, *Paul Scherrer Institute*

Online characterization of aerosol composition at the near-molecular level has recently become possible with the development of extractive electrospray ionization time-of-flight mass spectrometer (EESI-TOF), which is capable of detecting lightly oxygenated to highly oxygenated organic molecules (HOM) with minimal fragmentation. Good correlations between the EESI-TOF, aerosol mass spectrometer (AMS) and Filter Inlet for Gases and AEROSols (FIGAERO) measurements were observed in recent studies, but the ion-to-mass response factors in complex samples remain unaddressed.

In this study, we investigated the EESI-TOF sensitivity to a variety of secondary organic aerosol components, including monoterpene ozonolysis and OH-aromatic oxidation products. Seed particles were introduced as condensation nuclei to promote gas-to-particle partitioning. An AMS was used to quantify the inorganic seed and bulk organic aerosol mass concentrations. A VOCUS proton-transfer mass spectrometer (VOCUS-PTR) was used to quantify lightly-to-moderately oxygenated organic compounds in the gas-phase. Condensation sink was enhanced by increasing the seed particle concentration, driving gas-phase condensation and particle-phase growth. The EESI-TOF sensitivity can be derived from the relative changes in EESI-TOF and VOCUS-PTR signals.

The EESI-TOF was able to measure O₁ to O₉ oxidation products in the particle phase in response to seed particle injections. Comparison with the VOCUS-PTR indicates that the EESI-TOF has higher sensitivities towards more oxygenated organic species. Comparison with the AMS indicates that the EESI-TOF responds quantitatively to the inorganic seed particles. Results here demonstrate the EESI-TOF's potential to quantify individual species in complex samples without direct calibration using a chemical standard.

5IM.2

Laboratory Evaluation of Organic Aerosol Chemical Composition and Partitioning Measurements Obtained from High-Resolution Mass Spectrometers with Different Soft Ionization Schemes. MANJULA CANAGARATNA, Jordan Krechmer, Melissa Morris, Andrew Lambe, Francesca Majluf, Harald Stark, Kaspar Daellenbach, Megan Claflin, Archit Mehra, Chenyang Bi, Brian Lerner, Felipe Lopez-Hilfiker, Gabriel Isaacman-VanWertz, John Jayne, Douglas Worsnop, *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 can measure a high mass fraction of organic aerosols with high chemical resolution as well as high time resolution. Recently several techniques that combine soft-ionization with high-resolution mass spectrometry have been developed to address this need. Here, we utilize several of these soft-ionization techniques simultaneously in the laboratory to study SOA formed from anthropogenic precursors such as trimethylbenzene and catechol. The goals of this work are to combine these techniques to obtain a more complete characterization of the laboratory SOA and to compare and contrast the speciation capabilities of the various measurement methods. For this study we utilized a Filter Inlet for Gases and AEROSOLS coupled to a chemical-ionization mass spectrometer (FIGAERO-CIMS), a Vocus Inlet for Aerosols (VIA), and an extractive electrospray ionization inlet (EESI). We examine the influence of thermal decomposition, chemical fragmentation, and ionization selectivity on FIGAERO-CIMS, VIA and EESI-MS measurements. Additional volatility information obtained from the FIGAERO thermograms is also assessed. Overall, while each instrument observed many signals common with other instruments, instrument-specific biases were observed. The I-FIGAERO was biased towards more oxidized aerosol constituents, whereas the EESI-TOF treated more and less-oxidized aerosol constituents equally. Off-line measurements with gas chromatography (GC) and ion mobility spectrometry mass spectrometry (IMS-MS) are also utilized to obtain increased molecular-level identification obtained via isobaric and isomeric separation.

5IM.3

Ionization Efficiency of Evolved Gas Molecules from Aerosol Particles in a Thermal Desorption Aerosol Mass Spectrometer. YU IDE, Kento Uchida, Nobuyuki Takegawa, *Tokyo Metropolitan University*

Thermal desorption aerosol mass spectrometers (TDAMSs) with electron ionization are widely used to quantitatively measure aerosol chemical compositions. The physical and chemical mechanisms affecting the ionization efficiency of evolved gas molecules are not fully understood. We have performed laboratory experiments to investigate key factors affecting the ionization efficiency using a custom-made TDAMS. Ammonium chloride (NH₄Cl) and ammonium iodide (NH₄I) are used as test compounds. The ion signals originating from ammonia (NH₃) and hydrogen halide (HX) were measured by altering the geometric relationship between the ionizer and vaporization point. The ratio of ion signals of NH₃ to HX tended to increase with increasing the divergence angle of evolved gas plumes. Experimental results suggested that spatial broadening of gas molecules could be an important factor affecting the ionization efficiency. To interpret the experimental results, we have developed a numerical model for simulating the dynamics of gas molecules evolved from aerosol particles. The simulation model is composed of two main sections. The first section simulates the elastic collisions of the evolved gas molecules in a small region near the vaporization source (collision domain), where the mean free paths of the molecules are much shorter than those in the surrounding high vacuum environment. The second section simulates the free-molecular dynamics from the boundary of the first section to the ionizer. The ionization efficiencies of ammonia and hydrogen iodide molecules that evolved from NH₄I particles were evaluated. Our results suggest that the molecular collisions during the early stage of plume expansion and possible changes in the molecular velocities induced by these collisions could be an important mechanism affecting the observed variability in the ionization efficiency. However, the physical and chemical processes of the vaporization and ionization of aerosol particles in TDAMSs may be too complex to be quantitatively reproduced using simplified numerical models.

5IM.4

Online Molecular Analysis of Secondary Organic Aerosol Using Droplet Assisted Ionization. DEVAN E. KERECMAN, Michael J. Apsokardu, Yao Zhang, Murray Johnston, *University of Delaware*

Droplet Assisted Ionization (DAI) is an inlet ionization technique that allows for detection of intact molecular ions from preformed aerosol droplets. In our laboratory, DAI is performed by passing droplets through a temperature-controlled capillary tube that serves as the inlet to a Waters SYNAPT G2-S mass spectrometer. In this study, DAI is used to perform online molecular characterization of secondary organic aerosol (SOA) generated in a flow tube reactor by monoterpene ozonolysis. Previous work with DAI has determined the optimum operating conditions for a variety of test compounds. Ion formation depends strongly on droplet solvent composition and capillary temperature. Aqueous droplets give orders of magnitude higher signal intensity than dry particles or droplets consisting of other solvent compositions (Apsokardu, M. J. et al. *Rapid Commun. Mass Spec.* 2019). In the current study, SOA generated in the flow tube is size-selected with a differential mobility analyzer, aqueous droplets are formed by passing the aerosol through a condensation growth chamber, and sent into the DAI capillary inlet of the mass spectrometer to perform molecular analysis. In a previous study by our group using offline analysis to characterize β -pinene SOA, we noted a particle size dependence of the molecular composition, specifically an increasing oligomeric content with increasing particle size (Tu, P. and Johnston, M. V. *Atoms. Chem. Phys.* 2017). Presented here is an investigation of the size dependence on SOA composition using online analysis by DAI, as this method reduces the possible impact of artifacts associated with offline analysis. This work has implications for understanding the relative roles of gas- vs. particle- phase processes that cause particle growth.

5IM.5

Mechanism of Ion Formation by Droplet Assisted Ionization. MICHAEL J. APSOKARDU, Justin Krasnomowitz, Devan E. Kerecman, Yao Zhang, Shuai Jiang, Murray Johnston, *University of Delaware*

Droplet assisted ionization (DAI) has been developed for online molecular composition measurements directly from aerosol droplets. Analysis with DAI is done by passing droplets through a custom-built, stainless-steel capillary tube (69mm length; 1mm o.d.; 0.5mm i.d.) that has been interfaced with a Waters Synapt G2-S quadrupole ion mobility time-of-flight mass spectrometer. The DAI capillary has the option to be temperature-controlled between 25 and 850°C. Previous work has focused on determining the optimum conditions to maximize analyte ion signal intensities. One such factor is temperature of the capillary inlet, where a greatly enhanced signal is often seen at elevated temperatures. This temperature dependence provides a unique opportunity to examine the fundamentals of how gas phase ions are formed. Using the temperature dependence of absolute ion signal intensities, in combination with aerodynamic modeling of the capillary inlet, these data are reconstructed as an Arrhenius plot to give the activation energy (E_a) for ion formation. For the test compound polypropylene glycol, E_a is estimated to be 41.3 ± 3.1 kJ/mol. This value is not so different from the enthalpy of vaporization of water at 25°C, which is ~ 45 kJ/mol. Other test compounds give E_a values in the 30 to 40 kJ/mol range, indicating that the formation mechanism is strongly related to evaporation of water, but also depends on characteristics of the species being analyzed. Presented here are experimental measurements of E_a made with DAI in combination with theoretical calculations made by molecular dynamics simulations to understand the respective roles of solvent and analyte for producing ions from droplets. The results suggest that ions are ejected from the droplet surface into the gas phase with a surrounding cluster of water molecules. The water molecules are lost inside the mass spectrometer prior to mass analysis. Also, to be discussed are the implications of this mechanism to the application of DAI for online molecular characterization of aerosols.

5IM.6

Comprehensive Two-Dimensional Gas Chromatography Mass Spectrometry with Solid-state Thermal Modulator for In-situ Speciated Measurement of Organic Aerosols. ZHAOJIN AN, Haixia Ren, Mo Xue, Xiaosheng Guan, Jingkun Jiang, *Tsinghua University, China*

Thermal desorption aerosol GC/MS (TAG) is capable of online identifying speciated organics in atmospheric aerosols. Compared to reported quartz filter-based TAG (Ren et al. 2019a; 2019b), application of comprehensive two-dimensional gas chromatography increases resolution and sensitivity, mitigates unresolved complex mixture and co-elution, hence provides more accurate qualitative and quantitative information of organic aerosols. We report a quartz filter-based thermal desorption aerosol comprehensive two-dimensional GC/MS (2D-Q-TAG) which combines a solid-state thermal modulator with a quartz filter-based thermal desorption aerosol GC/MS. 2D-Q-TAG allows for in-situ automatic measurement of speciated organics in atmospheric aerosols with hourly time resolution. The solid-state thermal modulator conducts modulation independent of GC oven without using cryogenics or compressed air, which makes 2D-Q-TAG readily adaptive for field measurement. The system was evaluated using C7-C40 n-alkanes and 16 polycyclic aromatic hydrocarbons (PAHs). 2D-Q-TAG shows good performance with low limit of detection (LOD) of C13-C40 n-alkanes and 16 PAHs ranging from 0.001-0.104 ng. It was then deployed to measure structured chromatograms of ambient PM_{2.5} in Beijing. Less unresolved complex mixture and increased chemical resolution of this instrument can facilitate the characterization of atmospheric aerosol chemical composition.

[1] Ren et al., 2019a, *J Chromatogr A*, 1589: 141-148.

[2] Ren et al., 2019b, *J Chromatogr A*, in press (<https://doi.org/10.1016/j.chroma.2019.04.045>).

5IM.7

Isomer-resolved Chemical Characterization of the Particle-phase Oxidation Products of Indoor Emissions Using Gas Chromatography-Chemical Ionization Mass Spectrometry. CHENYANG BI, Graham Frazier, Jordan Krechmer, Wen Xu, Andrew Lambe, Megan Clafin, Brian Lerner, Manjula Canagaratna, John Jayne, Douglas Worsnop, Gabriel Isaacman-VanWertz, *Virginia Tech*

Oxidation of organic compounds emitted indoors produces hundreds or thousands of unique chemical components, both within and beyond the indoor environment into which they are emitted. The detailed arrangement of the atoms and structure of each individual compound (i.e. isomer-resolved composition) controls its chemical properties and effects. The substantial analytical challenge of characterizing this mixture has stymied a detailed understanding of chemical processes in indoor air. In this study, we developed a new instrument that quantifies known and previously unidentified compounds with resolution of individual isomers. A field-deployable Thermal desorption Aerosol Gas chromatograph was coupled to a time-of-flight Chemical Ionization Mass Spectrometer ("TAG-CIMS") using iodide as a reagent. The column effluent was also split to a flame ionization detector, providing near-universal responses to all analytes, and an electron ionization mass spectrometer, providing molecular structural information through fragmentation. This instrument measures molecular formulas of unknowns alongside identifications of known compounds and precise quantification of all analytes. We present here detailed characterization of the particle-phase oxidation products of common indoor emissions (e.g. limonene) over hours to days of atmospheric oxidation (by OH and O₃), with a focus on changes to particle composition as a function of aging. Furthermore, we present the directly measured sensitivity of the I-CIMS to a wide range of identified compounds and compare empirical sensitivity to currently adopted approaches to calibration (e.g. "voltage scanning"), yielding new insight into the capabilities and limitations of this reagent ion chemistry.

5UA.1**Variable Urban SOA Production Explained by Emissions and Photochemistry to Quantify its Impact on Mortality.**

BENJAMIN A. NAULT, Duseong Jo, Pedro Campuzano-Jost, Douglas Day, Weiwei Hu, Jason Schroder, James Allan, Manjula Canagaratna, Hugh Coe, Peter DeCarlo, Jessica Gilman, Patrick Hayes, Daven Henze, B. Thomas Jobson, Bill Kuster, Bernhard Rappenglueck, James Roberts, Jochen Stutz, Ezra Wood, Dominique Young, Bin Yuan, Brian McDonald, Joost de Gouw, Jose-Luis Jimenez, et al., *CIRES, University of Colorado, Boulder*

Secondary organic aerosol (SOA) is an important constituent of urban submicron aerosol around the world and one of the causes of poor air quality and premature mortality. However, urban SOA (USOA) sources and production remains poorly understood. We show that the production of USOA and gas-phase photochemical pollutants (Ox, HCHO, and PAN) across worldwide megacities (Beijing, Houston, London, Los Angeles, Mexico City, New York City and Boston, and Seoul) are strongly correlated to the emissions of specific types of volatile aromatic compounds (benzene, toluene, ethylbenzene, and xylenes). The differences in key USOA production metrics (normalized USOA concentration vs. time and USOA vs. Ox, HCHO, PAN) measured across these megacities are correlated with population density, and appear to be driven by differences in the relative importance of traffic and volatile chemical products as precursor sources. Using this observation, we provide one of the first nearly complete USOA mass closure for 7 different megacities on 3 continents by estimating IVOC emissions with 3 different methods. The observed relationships allow more accurate predictions of USOA, using the SIMPLE parameterization method, in the GEOS-Chem chemical transport model. We show that, globally, ~400,000 less premature deaths fewer year would occur if USOA precursors were regulated and removed.

5UA.2**Impact of Fireworks, Residential Wood Burning, and Wildfire on PM2.5 Concentrations in Southern California.**

XIANG LI, Melissa Sheffer, Mark Bassett, Scott A. Epstein, *South Coast Air Quality Management District*

The South Coast Air Basin (SCAB), which includes the Los Angeles metropolitan area and surrounding suburban areas, is home to approximately 17 million people and is considered one of the most polluted regions in the nation. Although PM2.5 concentrations in the SCAB have dropped significantly over the past two decades, high pollution events such as Independence Day fireworks, residential wood burning during Christmas and New Year holidays, and wildfires can still cause exceedances of the 24-hour PM2.5 federal standard.

PM2.5 concentrations and composition are measured throughout the SCAB with state-of-the-science regulatory and research-grade instrumentation. To study the contribution of these events to PM2.5 in SCAB in 2017 and 2018, we analyzed PM2.5 data measured by continuous Federal Equivalent Method (FEM) instruments, black carbon measurements from Aethalometers, and metal and other inorganics measurements from Cooper Xact instruments and X-ray Fluorescence (XRF) techniques. PM2.5 speciation data collected at the National Air Toxics Trends Station (NATTS) in central Los Angeles from 2012 to 2018 were also analyzed to examine the multi-year seasonal trend of organics, inorganics, metal, and elemental carbon in PM2.5 in the SCAB.

Preliminary results show that 1) PM2.5 speciation in firework emission-dominated days has distinct signatures compared to wildfire and residential wood burning emission-dominated days. 2) Metals comprise a much larger share of the total PM2.5 mass on firework days (~60%) than in wildfire and residential wood burning days (~10%). 3) On high PM2.5 days (larger than 35 $\mu\text{g}/\text{m}^3$) in winter, ammonia and nitrate often dominate (>60%) the total PM2.5 mass potentially due to higher humidity typically experienced in winter, which favors the formation of ammonia nitrate in the particle phase. 4) The relative contribution of inorganic and organic mass to total PM2.5 shows a strong seasonal variation with the strongest organic contribution occurring during the winter month.

5UA.3

Rethinking Near-road PM_{2.5} in US Cities. RAJ LAL, Anu Ramaswami, Armistead G. Russell, *Georgia Institute of Technology*

Emissions from mobile sources have historically been an important anthropogenic contributor to ambient air pollution leading to high levels of air pollution near major roadways. The US EPA recently implemented the Near-Road (monitoring) Network to measure NO₂ concentrations by high-traffic roadways in urban centers throughout the US, as these locations were believed to characterize worst-case human exposures to traffic-related pollutants. Many near-road sites also include CO and PM_{2.5} measurements, which along with the NO₂ observations, were compared against companion non-near-road monitors located within a 10 mile (~city scale) radius. Unexpectedly, we found no statistical difference ($\alpha = 0.05$) in PM_{2.5} concentrations between the near-road and non-near-road urban sites ($\delta = 0.33$ (-0.08-0.74) $\mu\text{g m}^{-3}$, $n=80$ comparisons), while NO₂ and CO levels, on average were significantly higher at the near-road sites versus the non-near-road urban sites by 5.5 (4.2-6.7) ppb and 0.10 (0.05-0.12) ppm, respectively. The average PM_{2.5} difference (~4%) is considerably lower than previously found, and in 31 of the 80 monitor comparisons PM_{2.5} is actually higher at the non-near-road urban sites relative to its near-road pair. Cleaner vehicle fleets, decreased formation rates in the near-road environment, the prevalence of other non-vehicular sources of emissions, the displacement of non-mobile sources in the near-road environment, and reactive PM transport wherein formation of secondary PM from on-road emissions occurs further downwind (i.e., away from the road) are likely responsible for this finding. Given that PM_{2.5} concentrations dominate air pollution-related health risks, these findings across 22 major US cities suggest we rethink our assumptions about elevated PM-related health risk exposures in the near-road environment.

5UA.4

Urban Atmospheric Aerosol Size Distributions: A Global Perspective. Tianren Wu, BRANDON E. BOOR, *Purdue University*

Measurements of aerosol particle size distributions (PSDs) have been widely conducted in the urban atmospheric environment. However, there is limited research summarizing and synthesizing such measurements in order to identify geographical variations in the shape and magnitude of number and mass PSDs. The objective of this study is to establish a comprehensive urban PSD database by analyzing urban PSDs measured in cities around the globe.

The urban PSD database contains $n=800$ PSDs measured over the past two decades in $n=124$ cities in $n=51$ countries. Urban PSDs are classified by region: Africa (AF); Central, South, and Southeast Asia (CSSA); East Asia (EA); Europe (EU); Latin America (LA); North America (NA); Oceania (OC); and West Asia (WA). Collectively, the PSDs span the nucleation to coarse modes (3 to 10,000 nm). Multi-lognormal fitting parameters for each number and mass PSD are provided to facilitate subsequent analysis by the aerosol research community. Several different multi-lognormal fitting strategies were utilized according to the different size ranges and measurement techniques. Details on the measurement conditions are provided. The electrical mobility diameter was used as the reference size definition for the database. A size-resolved urban aerosol effective density database was compiled to allow for accurate conversion between the number and mass PSDs and from aerodynamic to electrical mobility diameter.

Geographical variations in the shape and magnitude of urban PSDs were identified. Significant variations in urban number PSDs were found between cities in EU, NA, and OC with those in CSSA and EA. In general, number PSDs in EU, NA, and OC are dominated by nucleation (3 to 10 nm) and Aitken (10 to 100 nm) mode particles, while those measured in CSSA and EA are shifted to larger particles and tend to present a dominant peak in the accumulation (100 to 1,000 nm) mode. Urban mass PSDs in CSSA, EA, EU, NA, and LA are typically bi-modal, exhibiting a dominant peak in the accumulation mode and a secondary peak in the coarse (1,000 to 10,000 nm) mode, while those in WA often show a dominant peak in the coarse mode. Weighted median agglomerated normalized PSDs are provided for each region. Most urban PSD measurements were short-term, with only 14% providing data for > 6 months. There are a paucity of urban PSDs measured in AF, CSSA, and LA, demonstrating the need for long-term aerosol measurements across wide size ranges in many cities around the globe.

5UA.5

Air Quality in Canadian Port Cities: Regulation of Large Vessels to Low-Sulfur Marine Fuel in the North American Emissions Control Area (NA ECA). Angelos Anastasopoulos, Uwayemi Sofowote, PHILIP K. HOPKE, Mathieu Rouleau, Tim Shin, Ryan Kulka, Paul-Michael Farrah, Mark Gibson, *Health Canada*

Marine transportation can contribute significantly to air pollution levels in areas near commercial ports and seaways. This is a concern for many highly populated Canadian communities, such as Vancouver, Montreal, Halifax, and other coastal/seaway locations. Historically, large marine vessels have used bunker fuel oil, a low-grade diesel-type fuel with high sulfur (S) content associated with substantial releases of sulfur dioxide (SO₂) and components of fine particulate matter (PM_{2.5}) such as sulfate (SO₄²⁻) and heavy metals, as well as other combustion-related pollutants (NO_x, CO, VOCs), greenhouse gases (CO₂), and the formation of ground-level ozone (O₃). With growing awareness of the environmental and health impacts of marine shipping air pollution, Canada and the United States jointly designated a North American Emissions Control Area (NA ECA) and over the period 2012 to 2015 phased in lower-sulfur marine fuel regulations for large ships operating in coastal waters and ports. Health Canada has assessed ambient air quality at Canadian port cities on the Atlantic and Pacific coasts and along the St. Lawrence Seaway before, during, and after implementation of the NA ECA marine fuel regulations and also carried out comprehensive and targeted near-harbor and community air sampling campaigns before/after the regulations at the port city of Halifax. Findings are generally a 'good news story' and source-based analysis will be presented demonstrating the substantial and beneficial effect of the regulations on improving air quality with respect to SO₂ and, more moderately, PM_{2.5}. As such, Health Canada's research provides air health data that is highly meaningful to populations living near large ports and also addresses the broader issue of 'regulation accountability,' relevant to pending further regulation of marine fuel quality, such as the 2020 fuel sulfur cap for international waters.

5UA.6

Trends in PM_{2.5} Transition Metals in Urban Areas across the United States. CHRISTOPHER HENNIGAN, Aidan Mucci, Brian Reed, *University of Maryland, Baltimore County*

Many studies have characterized temporal trends in sulfate, nitrate, ammonium, and carbonaceous compounds – the major components of PM_{2.5} mass – across different regions of the U.S. However, due to their typically minor contribution to PM mass, atmospheric trends in transition metals have not been closely studied. We have characterized trends in PM_{2.5} transition metals in urban areas across the United States for the period 2001 - 2016. The metals included in this analysis – Cr, Cu, Fe, Mn, Ni, V, and Zn – were selected based upon their abundance in PM_{2.5}, known sources, and links to toxicity. Ten cities were included to provide broad geographic coverage, contrasting source influences, and climatology. The concentrations of V and Zn decreased in all ten cities, though the V decreases were more substantial. Cr concentrations increased in cities in the East and Midwest, with a pronounced spike in concentrations in 2013. The National Emissions Inventory (NEI) was used to link sources with the observed trends; however, the causes of the broad Cr concentration increases and 2013 spike are not clear. Analysis of PM_{2.5} metal concentrations in port vs. non-port cities showed different trends for Ni, suggesting an important but decreasing influence of marine emissions. The concentrations of most PM_{2.5} metals decreased in LA, STL, BAL, and SEA while concentrations of four of the seven metals increased in DAL over the same time. Comparisons of the individual metals to overall trends in PM_{2.5} suggest decoupled sources and processes affecting each. These metals may have an enhanced toxicity compared to other chemical species present in PM, so the results have implications for strategies to measure exposures to PM and the resulting human health effects.

5UA.7

Air Quality Management in Chile: Effectiveness and Environmental Justice Issues. HECTOR JORQUERA, Yasna Llanos, Ana Villalobos, Javier Ustariz, *Pontificia Universidad Catolica de Chile*

70% of Chile's population live in urban areas where ambient PM_{2.5} exceeds the annual ambient standard (AAQS) of 20 µg/m³. Cities in southern Chile (south of 35°S) suffer from severe air pollution coming from residential wood burning (Villalobos et al, 2017).

Government response is to generate Air Quality Management Plans (AQMP, PDA in Spanish), after an exceedance to an AAQS has been measured; then a set of initiatives are promoted. In cities where wood burning is a dominant source, measures such as a stove change out program, promoting dry wood sales and subsidies for housing thermal refurbishment are among the ones implemented by local authorities.

We assess the effectiveness of this Government policy by estimating trends in ambient PM_{2.5} in those southern cities that have implemented an AQMP, and compare them with close cities that do not have such a program.

Another issue is that smaller cities (population < 100,000 inhabitants) do not have ambient air quality monitoring, so they are not included in the aforementioned AQMP.

We analyze as case study the city of Molina (35.1°S, 71.3°W, population: 40,000 inhabitants) located 13 km south of Curicó (35°S, 71.2°W, population: 103,000 inhabitants) where ambient monitoring has been carried out by Government since 2012. We show results of a short-term ambient PM_{2.5} campaign carried out in winter 2018 with filters. We confirm that ambient PM_{2.5} concentrations in Molina are similar to those measured at Curicó, the closest city with routine ambient monitoring. Thus, Government policies ought to consider this environmental justice issue in the coming years.

References:

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- [2] A. M. Villalobos, F. Barraza, H. Jorquera, J. J. Schauer. *Environmental Pollution*. 225, 514–523 (2017).

6AC.1**Raoult was Right: A Fresh Old Look at Solution**

Thermodynamics. ANTHONY S. WEXLER, Ahmad Ikram, Simon Clegg, Devis Di Tommaso, Xiangwen Wang, *University of California, Davis*

In 1887, Raoult published his seminal work on the vapor pressure in mixtures stating that the vapor pressure is proportional to the mole fraction of the solute in solution. For dilute solutions, this relation holds but deviations grow as the solution becomes more concentrated especially in concentrated solutions. In 1908, Callendar proposed a simple and intuitive model of water activity as a function of solution composition and hydration number essentially extending Raoult's theory to more complex solutions where solute and solvent are associated. In 1973, Stokes and Robinson proposed a step-wise hydration model recognizing that the hydration number must decrease as the water activity decreases.

In this work, we derived analytical expressions for molality and solute activity as a function of water activity from infinitely dilute solutions to supersaturation, conditions that often prevail in atmospheric aerosols. We also derive expressions for the hydration number at infinite dilution that reproduces observations. Molecular dynamics simulations demonstrate the distribution of solute hydration which is also incorporated into the model.

6AC.2

Exploring Gelation in Model Marine Aerosol Particles: Micro-Rheological Observations of Ternary Water-Monosaccharide-Calcium Ion Microdroplets. RYAN DAVIS, David Richards, Kristin Trobaugh, *Trinity University*

Laboratory and field studies have demonstrated that atmospheric aerosols can exist as highly viscous liquids, semi-solids, and glasses. Such (semi-)solid particles are characterized by long timescales of equilibration with gas-phase species and slow diffusion of reactants throughout the particle bulk. Understanding the properties of semi-solid atmospheric aerosols is thus important to accurately represent aerosol water uptake and multi-phase chemistry in atmospheric models. In the past decade, a number of studies have characterized the rheological properties, such as viscosity, of model organic aerosols. These studies have shown many binary aqueous organics, such as aqueous sucrose, exhibit behavior consistent with viscous Newtonian fluids, with a predictable increase in viscosity upon decreasing relative humidity (RH). To date, studies have focused on those systems that exhibit such Newtonian behavior. However, it is known that marine-derived organic and inorganic material can potentially form Non-Newtonian fluids, such as gels; The behavior and properties of non-Newtonian gels remain understudied and it is unclear what aerosol compounds can form gels and under what conditions.

Here, using a dual-stage quadrupole trap as a micro-rheological tool, we present observations consistent with the formation of non-Newtonian gels in ternary microdroplets composed of aqueous monosaccharides and Ca^{2+} salts. For all of the monosaccharides studied, no gelation is observed in the binary monosaccharide nor ternary NaCl-monosaccharide systems, consistent with past studies. By contrast, in the presence of Ca^{2+} (i.e., in ternary CaCl_2 -monosaccharide systems), gel formation is observed as high as ~60% RH. Gelation is found to depend on the molecular functionality and stereochemistry of the monosaccharides, as well as the identity of the counter-anion of the salt. As will be discussed, these observations provide a conceptual basis to predict gel formation in mixed organic-inorganic aerosol.

6AC.3

The Effect of Molecular Weight on the Phase Separation of Polymer-Polymer Aerosol Particles. EMILY-JEAN OTT, Miriam Freedman, *The Pennsylvania State University*

The creation of core shell polymer aerosol particles often occurs by following typical nanoparticle synthesis methods and then aerosolizing the solution that contains the nanoparticles. We are able to create polymer aerosols directly from a solution, and the particles show predictable morphologies. We atomize solutions containing two water soluble polymers that are able to undergo liquid-liquid phase separation, rapidly dry the particles, and then impact them on carbon grids. The particles are then studied using cryo-transmission electron microscopy. The images are analyzed for particle area equivalent diameters and morphology. The polymers used in this study are polyethylene glycol (PEG) and dextran. By imaging submicron particles composed of these polymers with particle diameters as small as approximately 30 nm, we are able to determine that the particles exhibit a size dependent morphology. The larger particles undergo phase separation and exist in a core shell morphology, while smaller particles do not and maintain a homogenous morphology. We show that the region of particle sizes where morphology transitions from phase separated to homogenous can be tuned by changing the molecular weight of the polymers. We kept the monomer ratio between the PEG and dextran polymers approximately the same as we changed the molecular weights. In the molecular weight range studied, systems composed of low molecular weight polymers maintained a homogenous morphology in particles at larger sizes than systems composed of polymers with higher molecular weights. We are able to model this trend by using a system of equations that combine classical nucleation theory and Flory-Huggins theory. These morphology tunable aerosol particles could have potential applications in the pharmaceutical and sensor industries.

6AC.4

Spreading Ratio and Morphology of Size-dependent Secondary Organic Aerosols. ZIYING LEI, Nicole Olson, Yue Zhang, Yuzhi Chen, Andrew Lambe, Natalie White, Joanna Atkin, Jason Surratt, Andrew Ault, *University of Michigan*

Secondary organic aerosols (SOA), accounting for a large portion of the atmospheric particulate matter, are formed by oxidation of volatile organic compounds (VOC). VOC oxidation products either nucleate, condense, or undergo multiphase chemical processes that contribute to SOA mass loadings. Resolving the chemical complexity, morphology, and viscosity of SOA is crucial for understanding the impacts of atmospheric aerosols. Viscosity can be defined in terms of the spreading ratio of impacted particles. The chemical composition of particles and relative humidity (RH) both affect viscosity and need to be accounted for when determining and predicting aerosol particle spreading ratios. However, the viscosity of atmospheric particles is currently poorly quantified, and understanding the relationship between spreading ratios of size-selected aerosol particles and viscosity is still incomplete. Morphology also plays an important role in understanding atmospheric aerosols since it affects mixing state, heterogeneous chemical reactions, and optical properties, but is hard to quantify in SOA models due to complex chemical compositions and diverse ambient conditions.

This study investigated size-dependent spreading ratios and morphologies of four different types of SOA, such as toluene SOA, α -pinene SOA, isoprene SOA, and β -caryophyllene SOA. To determine spreading ratio as a function of particle chemical composition and size, laboratory experiments were conducted on four types of size-selected SOA particles (150nm, 200nm, and 250nm) at 50% RH. Atomic force microscopy coupled with infrared spectroscopy (AFM-IR) and Raman spectroscopy were used to characterize morphology, spreading ratio, and chemical composition of individual SOA particles. Results show that phase separation frequently occurred; specifically, core-shell and partially-engulfed morphologies were observed for the four types of SOA examined. Spreading ratios significantly changed as a function of the SOA precursor, which can be used to improve estimates of SOA physicochemical properties.

6AC.5

Dynamic Nature of the Particle Phase for SOA Derived from Select Green Leaf Volatiles. KEVIN FISCHER, Giuseppe Petrucci, *University of Vermont*

Secondary organic aerosols (SOA) are produced via gas phase oxidation reactions of volatile organic compounds (VOCs). Despite the integral role of SOA in atmospheric processes, there remains a limited understanding of the chemical and physical changes induced in SOA as it is formed and subsequently aged. The physical state of SOA is an especially important parameter, as it impacts SOA formation and growth, gas-particle partitioning, and reactive uptake on particle surfaces. Here, an Electrical Low Pressure Impactor (ELPI) was utilized to determine the bounce factor (BF; a surrogate for particle viscosity) as a function of reaction time for SOA derived from ozonolysis of *cis*-3-hexenyl acetate (CHA), *cis*-3-hexenol (HXL), and 1-octene-3-ol (OTL), all of which are green leaf volatiles (GLVs; a subset of VOCs) and have the potential to contribute significantly to the overall SOA budget. In addition, a Scanning Mobility Particle Sizer (SMPS) and Near-Infrared Laser Desorption-Ionization Aerosol Mass Spectrometer (NIR-LDI-AMS) were utilized to probe SOA concentration and chemical composition, respectively. An initially higher BF was observed (CHA: 0.17; HXL: 0.62; OTL: 0.63), followed by an immediate decrease after which the BF remained relatively constant (CHA: 0.038; HXL: 0.31; OTL: 0.32). Concurrently, SOA concentration and particle diameter continued to increase. Furthermore, addition of methanol as a stabilized Criegee intermediate scavenger led to lower BF values, lower SOA concentrations, lower particle diameters, and absence of expected SOA products. This suggests oligomers are initially formed and immediately partition to the particle phase, after which they act as nucleation sites for further SOA products to condense onto. This work provides direct evidence for the key role of the stabilized Criegee intermediate in the ozonolysis of the GLV systems studied and the dynamic nature of the particle phase during the SOA lifetime.

6AC.6

Effects of Water-soluble Organic Carbon on Aerosol pH. MICHAEL BATTAGLIA JR., Rodney J. Weber, Athanasios Nenes, Christopher Hennigan, *University of Maryland, Baltimore County*

Water soluble organic carbon (WSOC) is a ubiquitous and significant fraction of fine particulate matter. Despite advances in aerosol thermodynamic equilibrium models, there is limited understanding on the comprehensive impacts of WSOC on aerosol acidity (pH). We address this limitation by studying submicron aerosol that represent the two extremes in acidity levels found in the atmosphere: strongly acidic aerosol from Baltimore, MD, and weakly acidic conditions characteristic of Beijing, China. These cases are then used to construct mixed inorganic/organic single-phase aqueous particles, and thermodynamically analyzed by the E-AIM and ISORROPIA models (in combination with activity coefficient model AIOMFAC) to evaluate the effects of WSOC on the H⁺ ion activity coefficients (γ_{H^+}) and activity (pH). We find that addition of organic acids and non-acid organic species concurrently increases γ_{H^+} and aerosol liquid water. When allowed to modulate pH, these effects mostly offset each other, giving pH changes of < 0.6 pH units even if organics dominate aerosol dry mass (in excess of 60%). Surprisingly, non-acidic WSOC compounds were found to have a larger effect on pH than organic acids owing to their stronger impacts on γ_{H^+} . The model simulations were run at 70%, 80%, and 90% relative humidity (RH) levels and the effect of WSOC was inversely related to RH. At 90% RH, WSOC altered aerosol pH by up to ~0.2 pH units, though the effect was up to ~0.6 pH units at 70% RH. The offsetting nature of these effects suggests that aerosol pH is sufficiently constrained by the inorganic constituents alone and under conditions where liquid-liquid phase separation is not anticipated to occur.

6AC.7

Using Nitric Acid- Nitrate Partitioning and Aerosol Composition Data to Constrain Gas-phase Ammonia Levels and Aerosol pH. IFAYOYINSOLA IBIKUNLE, Rodney J. Weber, Athanasios Nenes, *Georgia Institute of Technology*

Atmospheric aerosol acidity drives multi-phase/heterogeneous chemistry, gas phase oxidant concentrations, secondary aerosol formation and particle composition. Aerosol acidity also drives the gas/particle partitioning of semi-volatile species (e.g., gas-phase ammonia - particle ammonium) which constitute a large fraction of particulate matter. At present, gas/particle partitioning and aerosol acidity (pH) are calculated most effectively through thermodynamic equilibrium models, among which include ISORROPIA II. To achieve the most accurate equilibrium model predictions, a full suite of ambient observations comprised of temperature, relative humidity, and total (gas + particle) concentrations are required as model input. However, a complete data set is often times unavailable. In-situ measurements of ammonia are challenging to acquire, and infrequent, whereas gas phase nitric acid and fine particle nitrate are more frequently measured. We have developed an algorithm based on ISORROPIA II that extends its functionality to infer ammonia concentrations using observed nitrate/nitric acid partitioning as a constraint for conditions where the inorganic aerosol is dominated by nitrate, sulfate, and ammonium. Given that observational data are uncertain, and ambient data does not always fully follow thermodynamic equilibrium, sensitivity tests using synthetic data show that ammonia inferences are most reliable under conditions where relative humidity is between 55-85%, and nitrate partitioning fractions are between 0.2-0.8. Preliminary findings from a field campaign in Korea during May- June 2016 resulted in ammonia estimations between 2-10 $\mu\text{g m}^{-3}$ (3-15 ppbv), which were deemed plausible based on CrIS satellite observations. Predicted pH primarily fell within the range of 1-3. Future work will focus on applying this new thermodynamic analysis to existing ambient datasets for development of thermodynamically-based inferences of ammonia concentrations, pH predictions, and ultimately, the state of atmospheric (aerosol) acidity.

6AC.8

Global Observations of Ammonium Balance and pH Indicate More Liquid Aerosol and Acidic Conditions than Current Models Predict. BENJAMIN A. NAULT, Pedro Campuzano-Jost, Douglas Day, Jason Schroder, Roya Bahreini, Huisheng Bian, Mian Chin, Simon Clegg, Peter Colarco, John Crouse, Jack Dibb, Michelle Kim, Jack Kodros, Felipe Lopez-Hilfiker, Eloise Marais, Ann M. Middlebrook, J. Andrew Neuman, John Nowak, Jeffrey R. Pierce, Eric Scheuer, Joel A. Thornton, Kostas Tsigaridis, Patrick Veres, Paul Wennberg, Jose-Luis Jimenez, *CIRES, University of Colorado, Boulder*

The inorganic composition of aerosol impacts numerous chemical and physical processes and properties. However, many chemical transport models show large variability in both the concentration of the inorganic aerosols and their precursors (up to 3 orders of magnitude differences) and the inorganic aerosol composition. Different models predict very different properties (e.g., aerosol liquid water concentration and aerosol acidity) and outcomes (e.g., heterogeneous uptake of gases or aerosols direct and indirect impacts on climate). Here, I use airborne observations from campaigns conducted around the world to investigate how the inorganic fine aerosol (PM₁) composition, and one of its key parameters, aerosol acidity, changes from polluted regions (Mexico City, Los Angeles, Northeastern US, and Seoul) to remote ocean basins (the Atmospheric Tomography campaigns 1 and 2) in order to provide constraints for the chemical transport models. I find that the empirical ammonium balance with major ions (ammonium balance = $\text{mol NH}_4 / (2 \times \text{mol SO}_4 + \text{mol NO}_3)$) rapidly decreases from 0.85 in polluted regions to less than 0.2 in remote regions, contradictory to some modeling studies that suggest most of the inorganic aerosol has a balance near 1. The data imply very low NH₃ in the upper troposphere, contrary to predictions of some models, implying different physical properties than predicted in models. Comparison of 9 chemical transport models show large variability for the ammonium balance compared to observations and a general high bias in the ammonium balance, likely due to underestimation of sulfate aerosol. This would imply different chemical and physical properties in the models than observed. Next, I explore the aerosol acidity with the E-AIM model, constrained by the observations, and find that the acidity increases from the most polluted/urban (median pH = 2.3) to most remote regions (median pH = -0.5). The chemical transport models have difficulty reproducing the aerosol acidity, showing both over and underestimation in pH. Several causes likely lead to these measurement vs model differences in aerosol acidity, including the mixing state of sea salt (internal vs. external), total amount of NH_x present in the atmosphere (NH_x = NH₃(g) + NH₄⁺(p)), and an underestimation of sulfate.

6BC.1

A Meta-Analysis of Black Carbon Emissions from Fire-Prone Ecosystems in the United States. ANDREW MAY, Hanyang Li, Robert J. Yokelson, Gavin McMeeking, *The Ohio State University*

Wildland and prescribed fires affect several ecosystems in the United States (US) including the montane forests and chaparral regions in the west and forests and coastal plains of the southeast. These fires can produce large amounts of atmospheric black carbon (BC), but BC emissions estimates are subject to large variability, because instruments that quantify black carbon are operationally different and any given fire is inherently unique. Some of our recent work has focused on constraining instrument differences, but here, our main interest is the “natural” variability of fires. We have sampled roughly 30 different journal publications to develop a dataset comprising both laboratory and field estimates of BC emission factors (EF_{BC}) derived from different techniques for the aforementioned ecosystems, including thermal-optical, light absorption, and incandescence.

There appears to be large variability in reported EF_{BC} values for these ecosystems in the literature with coefficients of variation ranging from 56% to 96% in the laboratory and 14% to 74% in the field. If we account for instrument differences, these ranges are only slightly different (57% to 77% and 14% to 78%, respectively), which is remarkable considering that we estimate the average relative difference between instrument to be roughly 45%. These results suggest that even though the relative difference between two measurement techniques may appear large, this effect may be dampened when compiling EF_{BC} values from different studies for use in emission inventories, and consequently, instrument differences may result in a relatively small contribution to overall uncertainty of fire-related BC in chemistry-climate models.

6BC.2

Chemical Fingerprinting of Particulate Organic Compounds in Fresh Smoke Produced from Burning Individual Western U.S. Wildland Fuels. COTY JEN, Lindsay Hatch, Nathan Kreisberg, Christos Stamatis, Yutong Liang, Robert Weber, John Battles, Scott Stephens, Robert York, Kelley Barsanti, Allen Goldstein, *Carnegie Mellon University*

Wildfires in the western U.S. are becoming larger and more frequent due to climate change and historical fire suppression. Smoke particles emitted from wildfires are composed of thousands of organic compounds that can vary based upon the fuel burned. The purpose of this study is to identify particulate chemical tracers in order to relate smoke composition to a specific fuel or fuel type. Chemical fingerprints were developed from molecular speciation of smoke particles collected during the FIREX campaign at the USDA Fire Sciences Laboratory (Missoula, MT). Western U.S. wildland fuels were burned individually and the emitted smoke particles were collected onto filters. Filters were analyzed using thermal desorption, online derivatization, and 2-dimensional gas chromatography with electron ionization (70 eV) or vacuum ultra-violet light (10.5 eV) high-resolution time-of-flight mass spectrometry. Emission factors of individual organic compounds were normalized to the measured total organic carbon emission factor. Compounds were considered part of the fingerprint for a specific fuel when their ratios exceeded two standard deviations relative to other fuels. These chemical fingerprints were then compared to smoke collected during two western U.S. wildland fires: low-intensity prescribed burning at a managed forest (Blodgett Forest, Georgetown, CA, Nov. 2017) and high-intensity wildfires in northern California (Santa Rosa County, CA, Oct. 2017). Fuels that were identified by their fingerprints, such as manzanita and coniferous rotten log, matched the plant inventory of the forest plots/region. These results indicate that the chemical fingerprints derived from detailed molecular speciation can be used to help determine the specific fuels that burned during wildland fires.

6BC.3

Impact of Fuel Type and Combustion Phase on the Chemical Composition of Particulate Matter Emissions from Wildland Fires. AMARA HOLDER, Johanna Aurell, Ingrid George, Brian Gullett, Venkatesh Rao, *U.S. EPA*

EPA's 2014 National Emission Inventory reports emissions by flaming and smoldering combustion phases. The mass fraction of each chemical constituent is derived from EPA's SPECIATE database, which does not account for combustion phase and represents a minimal range of fuel types. Particulate matter emissions have exhibited wide variation across combustion conditions and fuel types. However, limited data exist on the variation of the chemical composition of particulate matter emissions and almost no information is available on the trace elemental composition. While these elements are emitted at low concentrations, the large amount of smoke generated by fires makes them a significant source to the atmosphere.

In this work, both field and laboratory fire sampling for a range of fuels (southeastern pine, western pine, tallgrass prairie, and peat) was used to understand how fuel characteristics and combustion conditions impact particulate matter emissions. A range of combustion conditions in the field were achieved by sampling emissions near back burns, head fires, and smoldering fuels. In the laboratory, air flow, fuel structure, and fuel moisture were varied to obtain a range of flaming and smoldering conditions with the same fuel. Particulate matter emission factors were strongly correlated with modified combustion efficiency and increased over an order of magnitude for smoldering versus flaming conditions for a single fuel type (5 – 50 g/kg). The minor elemental composition (e.g., K, Cl, Zn) exhibited poor correlation with combustion conditions and appeared to be more dependent on fuel type. These results demonstrate that both the fuel type and combustion conditions govern the particulate matter emissions from wildland fires and need to be accounted for in emissions inventories.

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.

6BC.4

Investigation into Airborne-Based Smoke Marker Ratios and Brown Carbon from Wildfires in the Western U.S. during the WE-CAN Study. AMY P. SULLIVAN, Jakob Lindaas, Emily Fischer, Lauren Garofalo, Delphine K. Farmer, Sonia Kreidenweis, Teresa Campos, Jeffrey Collett, *Colorado State University*

Biomass burning is one of the main sources of water-soluble organic carbon (WSOC), organic carbon (OC), and brown carbon (BrC) aerosols. Therefore, it is important to be able to determine the contribution of biomass burning to the WSOC and OC concentrations. Smoke marker measurements provide one of the most common methods to make this determination. The key to this approach is that the ratio of the smoke marker to the total WSOC or OC concentration must be known at the source. But there is still much uncertainty in these smoke marker ratios, especially for biomass burning emissions from prescribed burning and wildfires. Therefore, as part of the WE-CAN (Western Wildfire Experiment for Cloud Chemistry, Aerosol Absorption and Nitrogen) Study we collected smoke marker, WSOC, and BrC data from aboard the C-130 aircraft as it flew through smoke from wildfires occurring in the Western U.S. in July-August 2018. Results were obtained by coupling one Particle-into-Liquid Sampler (PILS) with a Total Organic Carbon analyzer for real-time measurement of BrC and WSOC and a second PILS to a fraction collector to provide off-line samples for smoke marker analysis by high-performance anion-exchange chromatography with pulsed amperometric detection. Airborne results from these measurements for a number of different wildfires will be presented. Smoke marker ratios from controlled laboratory burn source samples collected at the Fire Science Lab in Missoula, MT during the FLAME (Fire Science at Missoula Experiment) studies as well as samples collected from various prescribed burns and wildfires across the U.S. will be compared to the results from the WE-CAN measurements. How parameters such as aging and fuel type might play a role on smoke marker ratios and BrC will also be discussed.

6BC.5

Chemical Composition of Brown Carbon in Tar Ball Aerosols from Biomass Burning. Anusha P.S. Hettiyadura, Chunlin Li, Quanfu He, Yinon Rudich, ALEXANDER LASKIN, *Purdue University*

Biomass burning (BB) is a major source of brown carbon (BrC) aerosols. BrC causes adverse health effects and alter Earth's radiative energy balance by absorbing and/or scattering solar radiation or by acting as cloud condensation nuclei. Tar balls, which are submicron sized spherical carbonaceous particles, contribute to a significant fraction of BB BrC. This study explore the chemical composition of BrC in extracted tar ball materials, giving molecular insights to their light absorbing properties. Tar material was generated by heating and dry distilling wood pellets simulating oxidative (in the presence of air) and pyrolysis (in the absence of nitrogen) conditions. The separated aqueous and oil phases were diluted with acetonitrile and analyzed in reversed-phase liquid chromatography coupled with a photodiode array (PDA) detector and a high-resolution Orbitrap™ mass spectrometer (MS). Prior to MS detection the analytes were ionized using either electrospray ionization (ESI) or dopant-assisted atmospheric pressure photo ionization to detect both polar and nonpolar analytes, in both positive and negative ion modes. More than 90% of the organic compounds identified in tar balls were detected in ESI, indicating that most of these compounds contain polar functional groups. A total of 35 common chromophores were detected in all 4 samples. Oil phase samples showed additional chromophores that were retained longer on the column, indicating the presence of nonpolar chromophores in the oil phase compared to the aqueous phase. Furthermore, pyrolysis oil phase displayed more longer-retained chromophores compared to the oxygenated oil phase, reflecting their molecular differences. The light absorbing chromophores identified in this study serve as tracers for BB BrC in the atmosphere and further studies on their light absorbing properties will enable determining their effect on climate forcing.

6BC.6

Optical, Physical, and Chemical Properties of Emissions from Open Combustion of Cheatgrass (*Bromus Tectorum*). MEGAN RENNIE, Vera Samburova, Deep Sengupta, Andrey Khlystov, Hans Moosmuller, *Desert Research Institute*

Cheatgrass (*Bromus tectorum*) is a non-native, invasive annual grass species in the U.S. Intermountain West (USIMW) that plays an important role in fire ecology. Its increasing presence has created higher fuel loads that greatly amplify the frequency and extent of rangeland fires. Open areas where shrubs and desert grasses were once separated by areas of open soil are now connected through cheatgrass growth. Many studies have been conducted on the ecological effects of cheatgrass as an invasive species in the USIMW, yet next to nothing is known about optical, physical, and chemical properties of emissions from cheatgrass fires as needed for better estimating radiative forcing and understanding health effects. Cheatgrass burns primarily in the flaming combustion phase where large amounts of black carbon aerosols are emitted. These emissions contribute to air pollution events, affect the radiative budget and climate change, and can cause severe health effects.

Laboratory open combustion of cheatgrass was performed in the biomass combustion chambers of the Desert Research Institute to determine fuel-based emission factors and the physical and chemical properties characterizing the emissions of black carbon and other combustion aerosols. Our research also characterizes the physical properties of the emitted aerosols including size distribution, shape, and morphology as needed for a process-based understanding of particle optics, transport, and deposition. Additionally, the chemical composition of emitted aerosols will be determined as needed for a better understanding of the physical properties and toxicology that affect health impacts. These measurements will be analyzed to provide data essential for the modeling of radiative forcing and health impacts of cheatgrass fire emissions.

6BC.7

Chemically Distinct Emissions from Highly Controlled Pyrolysis of Three Wood Types. ANITA AVERY, Mariam Fawaz, Leah Williams, Tami Bond, Timothy Onasch, *Aerodyne Research, Inc.*

Wood pyrolysis contributes to biomass and biofuel burning emissions while being a distinct phase from flaming combustion. To isolate and study the processes and emissions of pyrolysis, a custom-made reactor was used to uniformly heat small blocks of wood under nitrogen. Small (max 154 cm³) pieces of maple, Douglas fir, and oak wood were pyrolyzed in a temperature-controlled chamber at 400, 500, or 600 C. The mass of wood lost during pyrolysis was measured in situ gravimetrically, gas phase CO was measured, and aerosol emissions were measured with an Aerodyne aerosol mass spectrometer (AMS) and a TSI Engine Exhaust Particle Sizer (EEPS). Gas and particle emissions increased rapidly after inserting a wood sample, remained high for tens of minutes, and then dramatically dropped off, leaving char behind. The particulate mass and chemical compositions (i.e., mass spectra) varied with experiment time, wood type, and chamber temperature. The emitted particles consisted primarily of low O:C organic matter, as measured by the AMS. Unlike flaming wood combustion, the oxygen poor pyrolysis organic emissions were dominated by small, singly oxygenated fragments including CO⁺ and CHO⁺, which together made up approximately 30-45% of the total aerosol mass, whereas CO₂⁺ accounted for less than 3%. Typical biomass burning marker ions, such as C₂H₄O₂⁺ at m/z 60, were significantly (~2X) more abundant than published literature for flaming combustion. Large unsaturated hydrocarbons were emitted with increasing abundance near the end of an experiment. These observations are reflective of the complex chemical processes occurring as each wood piece heats from the surface to core and thermally decomposes, and will be compared and contrasted with previous flaming combustion results. These results will help inform models of pyrolysis.

6BC.8

The Ubiquity of Biomass Burning Particles in the Global Remote Troposphere. GREGORY SCHILL, Karl D. Froyd, Daniel Murphy, Christina Williamson, Agnieszka Kupc, Charles Brock, Huisheng Bian, Mian Chin, Peter Colarco, Eric Ray, Alan Hills, Rebecca Hornbrook, Eric Apel, *NOAA ESRL and CIRES, University of Colorado Boulder*

Wildfires and open burning emit ~2.8 Tg of black carbon (BC) and ~31 Tg of primary organic aerosol (POA) every year. These estimates correspond to ~40% of global BC and ~60% of global POA emissions, with larger contributions if solid-fuel heating and cooking are included. Thus, biomass burning aerosols have immense potential to affect the Earth's climate system via both the aerosol direct and indirect effects. Despite this importance, there are few observational constraints on the global abundance of biomass burning particles. In particular, in-situ measurements in the global remote troposphere, far from biomass burning emissions, are almost entirely absent.

In this work, we provide the first seasonally resolved, global maps of biomass burning aerosol abundance from aircraft observations. Measurements were taken during the NASA Atmospheric Tomography (ATom) mission during 2016-2018. During ATom, nearly continuous altitude profiles (~0.15 to 12 km) of single-particle composition were measured by PALMS from 86°S to 82°N, primarily over the remote oceans. Despite oftentimes being thousands of km from biomass burning sources, we find that biomass burning particles make up 12-50% [interquartile range (IQR)] of the accumulation mode particle number and 11-40% (IQR) of the aerosol mass from 2 to 8 km in the remote troposphere. Comparisons of ATom observations to the GEOS-5 model indicates biomass burning aerosol wet removal processes are underestimated. Using an updated model, we estimate the climatic significance of biomass burning in the remote troposphere. We find that, on a monthly average, 37-68% of the AOD from biomass burning (globally summed) can be attributed to this ubiquitous smoke outside of defined biomass burning plumes.

6HA.1

Glottis Opening Effects on Inhaled Particle Deposition in Human Airways. TED SPERRY, Yu Feng, *Oklahoma State University*

The objective of this study is to determine the influence of glottis opening on the pulmonary airflow and inhaled particle deposition patterns in a subject-specific human respiratory system. The glottis, or opening between the vocal cords within the larynx, has the narrowest passage in the upper respiratory system which may significantly influence transport and deposition of inhaled particles. Humans are exposed to aerosols from manufacturing, mining, construction, and pollution which produce airborne particles that may be inflammatory, carcinogenic, or carry infectious diseases into the subject airways. Using an experimentally validated computational fluid-particle dynamics (CFPD) model, this study focuses on the variability between three cases of identical bronchial trees with glottis opening areas of 83, 126, and 254 mm² to explore the variations in airborne particle exposure risk. This study uses the Shear Stress Transport (SST) model to simulate the laminar-to-turbulent transitional airflow patterns with steady-state inhalation condition, then uses the Euler-Lagrange method to track particles. Specifically, these models reflect an inhalation rate of 30 L/min and introduce 100,000 particles with diameters of 0.5 μm for the first case and 2 μm for the second case. To isolate the effects of the glottic opening, the complex geometry of the mouth front was replaced by an idealized 20-mm circular inlet, which is identical for all cases. Numerical results indicate that glottis opening has a significant effect on local and regional particle deposition patterns, with the smaller glottis openings causing significant local deposition of inhaled particles when compared to that of the larger openings. Simulation results also suggest that future CFPD modeling efforts should realistically represent the glottis openings and dynamic motions to enable more accurate predictions of the flow patterns created by this structure and the resulting effects on particle deposition.

6HA.2

Oxidative Potential of Particulate Matter and Generation of Reactive Oxygen Species in the Epithelial Lining Fluid. TING FANG, Pascale Lakey, Rodney J. Weber, Manabu Shiraiwa, *University of California, Irvine*

Reactive oxygen species (ROS) play a central role in oxidative stress and possibly adverse health effects of atmospheric particulate matter (PM). Respiratory particle deposition can lead to the release of ROS in the epithelial lining fluid (ELF) due to catalytic reactions of PM redox-active components including soluble transition metal ions and organic compounds with lung antioxidants. Ambient particles with aerodynamic diameters below 2.5 μm as well as size-segregated particles (from 56 nm to 18 μm) were collected in Atlanta. Organic carbon and water-soluble metals were measured and PM oxidative potential was quantified with the dithiothreitol (DTT) and ascorbic acid assays. The kinetic multi-layer model of surface and bulk chemistry in the ELF combined with a human respiratory tract model was applied to estimate the concentrations and production rates of ROS by redox reactions of PM components. The extrathoracic region was found to have higher ROS concentrations compared to the bronchial and alveolar regions due to higher particle deposition into the ELF with lower ELF volume. Fe and Cu ions contribute mainly to H₂O₂ and O₂⁻ production rates, which show strong correlation with measured oxidative potential. In contrast, oxidative potential does not exhibit significant correlations with OH production rates, which are mainly driven by decomposition of secondary organic aerosols and Fenton(-like) reactions of metal ions. Oxidative potential is a good indicator of production of H₂O₂ and O₂⁻, but does not represent OH generation in the ELF. Combination of field measurements of chemical composition and oxidative potential with model simulations can provide critical insights into ROS formation by ambient PM in the human respiratory tract.

6HA.3

Time-Resolved Single Cell Response of Intracellular Reactive Oxygen Species to Aerosol Particles. FOBANG LIU, Josh Whitley, Nga Lee Ng, Hang Lu, *Georgia Institute of Technology*

Particulate matter (PM) exposure is a leading global human health risk. Adverse PM health effects have been proposed to be linked to oxidative stress through the generation of reactive oxygen species (ROS). Currently, most assays for cellular response measurement are low resolution (e.g., no single-cell information; not much temporal information), imposing limitations on our understanding of what components or characteristics of PM best account for its toxicity. In this study, we design and optimize microfluidic cell-trapping devices that allow for the long-term culture and imaging of single cells. For method validation, we employ the same bulk intracellular ROS assay (murine alveolar macrophages; fluorescent ROS probe: carboxy-H₂DCFDA) that we developed in our previous work. The average cellular ROS response of single-cell measurements is compared with the bulk cellular ROS data obtained via microplate reader. We find that the average data from single cell measurements are higher than that of the bulk data. This could be due to stagnant PM extracts in the well plates having a smaller impact than the continuously perfused PM extracts of the microfluidic device. Furthermore, we link the behaviors of cellular heterogeneity in ROS response to the chemical properties (e.g. oxidation state) of PM. Overall, this study describes a novel approach to understand cellular ROS generation over time at the single-cell level. Our work can serve as a proof of principle study to investigate a wide array of single-cell responses (beyond ROS) upon exposure to any types of PM.

6HA.4

Formation of Metal-Ligand Complexes in Atmospheric Aerosol and Their Effects on ROS Production in a Surrogate Lung Fluid. CHIARA GIORIO, Sara D'Aronco, Alessandro Negro, Valerio Di Marco, Andrea Tapparo, *Università degli Studi di Padova, Italy*

Aqueous phase processing of aerosol can lead to substantial modifications of aerosol chemical and physical properties. A process potentially very important in this context is the formation of metal-organic ligand complexes in atmospheric aqueous phases, like fog/cloud droplets and deliquescent aerosol. Such process can increase the solubility of metals, therefore their bioavailability, and affect their capability to generate reactive oxygen species (ROS). We investigated the formation of metal-organic ligand complexes, especially those involving small dicarboxylic acids, in urban aerosol collected at an urban background site in the city centre of Padua (Italy), in the Po Valley. We assessed the effects of metal-ligand complexes formation on the solubility and solubilisation kinetic of metals from the particles to aqueous solutions simulating fog/cloud water and a model pulmonary fluid. Preliminary results show that iron, copper and manganese are present in the aerosol in a complexed form, mainly with oxalate, malonate and succinate. Iron was the metal whose solubility was the most influenced by the presence of organic ligands. Solubilisation kinetics of many metals depended on the form in which they are present in the aerosol and they were influenced by the environmental conditions during the campaign. Changes in particle toxicity due to the formation of metal-ligand complexes was investigated in a model pulmonary fluid specifically developed to simulate the metal-ligand equilibria that might be established in a real pulmonary fluid. The ability of particles to generate ROS was tested based on the oxidation kinetic of glutathione and ascorbic acid to assess whether the formation of metal-ligand complexes increase or decrease particle toxicity.

6HA.5

Aerosol-mediated ROS Production: Roles of Functional Groups and Reaction Kinetics. HUANHUAN JIANG, Jin Chen, C.M. Sabbir Ahmed, Zixu Zhao, Haofei Zhang, Ying-Hsuan Lin, *University of California, Riverside*

The toxicity of organic aerosols has been largely ascribed to the generation of reactive oxygen species (ROS), which could subsequently induce oxidative stress in biological systems. Dithiothreitol (DTT) assay is an acellular assay widely used to determine the oxidative potential (the ability to generate ROS) of different types of PM at a laboratory benchtop scale. Both inorganic (i.e., transition metals) and organic species (i.e., quinones, organic hydroperoxides and electron deficient alkenes) in PM have been recognized as the main contributors to DTT responses. Conventionally, the reaction of DTT with redox-active species in PM has been assumed to be pseudo-first order, and the oxidative potential of PM is represented by the DTT consumption per minute of reaction time per μg of PM. However, inconsistency of DTT results among different studies has been reported. Recent studies have shown that the DTT consumption rate of PM decreased significantly with reaction time, which highlights the necessity of taking the reaction kinetics and mechanisms of DTT assay into consideration when interpreting DTT results. In this study, we investigated the reaction kinetics of DTT with model organic compounds with various functional groups. We observed that the DTT consumption rate largely depends on the initial sample and DTT concentrations. The reaction order of DTT with non-catalytic reactive species (e.g., conjugated carbonyls and organic hydroperoxides) is higher than first order. The reaction of DTT with different functional groups have significantly different rate constants. A predictive multiple linear regression model is developed to estimate the contributions of aerosol functional groups to oxidative potential using the measured reaction rate constants. This model will be applied to the DTT measurements of primary (e.g., e-cigarette smoke particles and diesel exhaust particles) and secondary organic aerosols (e.g., isoprene and toluene SOA). This study will provide molecular insights into the interpretation of DTT-based aerosol oxidative potential.

6HA.6

The Toxicity of Gasoline Automobile Engine Emissions Depends on Fuel Type (Gasoline and Ethanol) and Driving Cycle: A Combined Biological and Aerosol Composition Study. Sebastian Oeder, J. Candeias, Tamara Kanashova, Benjamin Stengel, M. Dilger, S. Murugadoss, Olli Sippula, Sebastiano di Bucchianico, S. Bauer, Thorsten Streibel, Martin Sklorz, Jürgen Orasche, Toni Miersch, Hendryk Czech, C. Rüger, Bert Buchholz, C. Weiss, Jorma Jokiniemi, Maija-Riitta Hirvonen, Gunnar Dittmar, C. Schmidt-Weber, Jeroen Buters, RALF ZIMMERMANN, HICE consortium, *University of Rostock and Helmholtz Zentrum Munich, Germany*

Car engine emissions are relevant for local air pollution and contribute to the greenhouse gas-burden. Therefore, the change from fossil- to renewable fuel-sources is promoted. The impact of the changing emission on human health, however, is widely unknown. Our study compares lung cell responses towards the exposure to diluted car engine emissions from engine-operation with conventional versus bio-fuel (ethanol). Also different driving cycles are considered. A standard 2.0 litre flexi-fuel engine with 132 kW/320 Nm was operated with gasoline containing either ~10% (E10) or ~85% (E85) ethanol. The NEDC and a high-speed driving cycles were used to simulated chassis dyno tests by operating the test bench engine with correlating speed/torque patterns. A lung epithelium cell line (A549) was directly exposed at the air-liquid-interface (ALI) to diluted (1:10, 1:40) emissions. After 4h of exposure cells were lysed, RNA extracted and analysed by whole-genome gene expression arrays. Using clean air treated cells as control, aerosol-induced gene regulation was calculated. Gene ontology (GO) and canonical pathway analysis was performed using at least 1.5-fold regulation and $p < 0.05$ in t-test with multiple testing correction. The cells reacted to the E85 emissions with a 2-fold increase in regulated genes compared to conventional fuel emissions. In the high-speed cycle (gasoline) the number of affected genes increased by 28% with respect to the standard NEDC cycle. All tested aerosols caused general cell-stress, affected the cell-cycle and inflammatory responses (GO term analysis). Canonical pathway analysis revealed additionally aerosol specific effects: Emissions from conventional gasoline caused higher levels of oxidative stress and fibrosis-related changes, whereas E85 emissions induced stronger DNA-damage responses (likely due to higher aldehyde concentrations in E85-emissions). We conclude that addition of higher amounts of ethanol may increase the emission's toxicity.

6HA.7**Collection Methods Affect the Physicochemical Properties of Combustion Particles and Their Cellular Response in a Human Macrophage-Like Cell Line.** KAMALJEET KAUR, Isabel C.

Jaramillo, Raziye Mohammadpour, Anne Sturrock, Hamid Ghandehari, Chris Reilly, Robert Paine, Kerry Kelly, *University of Utah*

A vast majority of in vitro studies expose cells to combustion-derived particulate matter (cdPM) in a suspension, which requires a method to collect cdPM and subsequent resuspension in an aqueous media. The consequences of different particle collection methods on particle physicochemical properties and resulting cellular responses are not fully understood. This study compared the physicochemical properties and cellular response in human macrophage (THP-1) for cdPM collected by three different methods. These collection methods included two common approaches (collection on a 200-nm PTFE filter followed by resuspension in DI water, and collection on a cold plate followed by scraping and resuspension in DI water) and one relatively new (direct bubbling in DI water) approach. All approaches used cdPM produced from a jet-fuel surrogate burned in a flat-flame burner under constant combustion conditions. The three approaches yielded cdPM with differences in particle size distribution, surface area, the presence of dissolved species, and oxidative potential. Among the collection methods, only the directly bubbled sample retained the bimodal distribution observed in the gas-phase. The directly bubbled sample suspension had the smallest mean radius (root mean square, rms, of 48.7 nm), followed by filtered (57.4 nm) and scraped (85.0 nm) sample. The bubbled sample contained ~50 % of its total mass as dissolved species and lower molecular weight compounds that were not found in the other two samples. These differences in the cdPM physicochemical properties affected the biological responses in THP-1 cells. The bubbled sample showed greater oxidative potential and cellular reactive oxygen species. The scraped sample induced the greatest inflammatory response (TNF α secretion). These findings have important implications for in vitro studies of air pollution and for efforts to better understand the underlying mechanism.

6HA.8**Quantitative Assessment of Organic Compound Deposition in the Human Respiratory System from Rechargeable E-Cigarettes.** YUAN SHAO, Kirsten Koehler, Ana Rule, Wentai

Luo, Kevin McWhirter, Jim Pankow, *Johns Hopkins Bloomberg School of Public Health*

To better understand exposure to inhalation hazards from e-cigarette aerosols, it is important to characterize the particle size-specific deposition in human airways. A foam sampler has been developed to capture the fraction of aerosols that deposits in the human respiratory system as a function of particle size. The objective of this study was to simulate e-cigarette vaping, and to quantify the fraction of organic compounds deposited in the human respiratory tract. We evaluated aerosols generated by JUUL devices (Virginia Tobacco flavor) using foam lung deposition samplers (LDS). An automated e-cigarette aerosol sampling system was designed for this study. E-cigarette emissions were generated at a flow rate of 4 LPM for 3 seconds with a 30-second break between puffs. The emissions were pulled through the LDS and the fraction of aerosol not collected in the LDS was collected with a 25mm Teflon filter to represent the exhaled fraction. JUUL samples were collected with 0, 20, 40 and 60 puffs per sample, each with 5 replicates. Total concentrations of Propylene Glycol (PG), Nicotine, and Glycerin (GL) in the LDS and filters were analyzed using GC-MS. The median mass collected in the LDS was 168.8 ug/puff for PG; 31.3 ug/puff for Nicotine, and 353.2 ug/puff for GL. The resulting median percentage of mass depositing in the lungs was 60% for PG; 60% for Nicotine, and 44% for GL. E-cigarettes are a source of hazardous organic compounds. We found that about half of the total inhaled mass was collected in the lung deposition sampler, indicating that compounds reach and nearly 50% deposit in the human respiratory tract during e-cigarette use. Additional studies are needed to evaluate the deposited mass for other popular e-cigarette devices and flavors.

6IM.1**Extending the Stolzenburg DMA Transfer Function to the Scanning Electrical Mobility Spectrometer (SEMS).**

YUANLONG HUANG, John Seinfeld, Richard Flagan, *California Institute of Technology*

The differential mobility analyzer (DMA) has been widely used in particle size distribution measurement. To increase the measurement time resolution, the high voltage applied to the DMA is ramped exponentially (SEMS) rather than stepped through a sequence of discrete voltages. The transfer function for this scanning DMA describes how counts of particles of a given size are distributed among the successive time bins after classification within the time-varying electric field of the DMA. While a transfer function has previously been derived for the scanning DMA in the limit of non-diffusive particles, diffusional effects, which are very important for particles at the lower end of the sizing domain, have only been taken into account through numerical simulation, often at a high computational cost. The Stolzenburg analysis that considers diffusion of particles from the ideal, nondiffusive trajectories provides a good approximation to the diffusional transfer function for a DMA that is operated at constant voltages. Here, we extend that method to scanning-mode operation of the cylindrical DMA. The kernel of this semi-analytical method is a contour plot of particle's residence time distribution inside the DMA in the inlet-outlet space, from which one can estimate the contribution of diffusion to particle transmission from inlet to outlet along different particle trajectories. This analysis reproduces the Stolzenburg transfer function in the asymptotic limit of constant-voltage operation. The scanning DMA transfer function derived by this method is further validated by comparison with that calculated by numerical simulations. By mapping the transmission probability between particle entrance and exit trajectories within the DMA, this semi-analytical method enables rapid calculation of both static and scanning DMA transfer functions for idealized DMA geometries; when applied to numerical simulations of nondiffusive trajectories, it further facilitates efficient determination of transfer functions with real DMAs.

6IM.2**The Role of Size Distribution Representation in Aerosol Data Inversion.**

RICHARD FLAGAN, Amanda Grantz, Yuanlong Huang, *California Institute of Technology*

Recovery of the particle size distribution from aerosol measurements involves: (i) the transfer function that describes the signals produced by particles of different sizes over the size range of the measurement; (ii) an algorithm for extracting a set of parameters that characterize the particle size distribution; and (iii) a mathematical representation of the particle size distribution. The transfer function is generally based upon empirical characterization of the instrument, or a theoretical model of the instrument that may be combined with empirical corrections that account for deviations of the real instrument from an idealized model. The best-studied measurement system is the differential mobility particle sizer (DMPS). The scanning electrical mobility spectrometer (SEMS or SMPS) has recently been advanced to similar fidelity through detailed numerical models of the real instrument. Algorithms for inverting the signals range from ad hoc successive approximation methods such as the Twomey algorithm, direct matrix inversion, least-squares and non-negative least-squares methods, and constrained regularization, among others. The representation of the particle size distribution has received less critical attention than the first two components of the data inversion problem. They include multi-modal log-normal representations, nodal (δ -function) representations, histograms or linear splines. Many papers fail to even mention which representation is being employed. Different size distribution representations impact the fidelity of data inversion. We simulate measurements to quantify biases and sources of uncertainty introduced during data inversion. The results reveal increased uncertainty when the size distribution extends beyond the measurement range of a single instrument, and that the magnitude of that uncertainty depends strongly upon the representation of the size distribution that is employed. We further demonstrate ways to reduce that uncertainty without increasing the number of parameters required to represent the size distribution, using codes that will be released open-source.

6IM.3

Asynchronous Functional Reactive Programming for Data Acquisition and Instrument Control: Example of a Free Software Implementation for Operating Scanning Mobility Particle Sizers. MARKUS PETTERS, *North Carolina State University*

Professional societies and funding agencies are moving towards open data policies that require publication of raw data and computer software used to generate results. Consequently, instrument control and data acquisition (DAQ) software ought to be shared with publication. Most manufacturers only distribute proprietary code in binary format with their instruments. Research groups that build new instruments often use proprietary special-domain languages such as LabVIEW to implement the DAQ software. Both models are unsuitable for publication and difficult to evaluate for correctness. Furthermore, DAQ software design principles are rarely debated in the scientific literature, thus slowing advances in instrument development. Here I show that functional reactive programming principles are well suited to construct reliable, efficient, and concise code for data acquisition and instrument control. The approach uses a textual syntax with a functional programming style, signal-based data structures, asynchronous event processing, and interfaces with a graphical user interface. To demonstrate the utility of the approach, free software to operate differential mobility analyzers (DMA) in scanning mode for size distribution measurement is shared. The code controls the instrument and acquires multiple data streams at two frequencies using a multifunction DAQ device and serial communication on a Linux platform. Raw DMA response functions are inverted in real time using the methodology described in Petters (2018, AS&T, doi:10.1080/02786826.2018.1530724). With moderate financial and time investment, the software can be used as is to operate a complete scanning mobility particle sizer system using a DMA column, high-voltage power supply, and detector. The software can log multiple auxiliary sensors and be adapted to build more elaborate programs controlling tandem DMA setups with complex duty cycles. The software design principles are general, portable to several common programming languages, and can be applied to a wide range of instrument automation scenarios.

6IM.4

MAGIC Spider: A Fast, Compact Scanning Electrical Mobility Spectrometer for UAV Deployment. STAVROS AMANATIDIS, Steven Spielman, Gregory Lewis, Susanne Hering, Richard Flagan, *California Institute of Technology*

Obtaining accurate particle size distributions aloft, especially in the ultrafine size range, is a challenge when power and weight are limited. Unmanned Aerial Vehicles are used increasingly to map atmospheric aerosols aloft, and in remote areas, but payloads are limited. To meet this need we have developed a new, highly portable mobility-based particle sizer. Our instrument, the “*MAGIC Spider*”, combines the “*Spider DMA*”, a compact radial-flow differential mobility analyzer designed by Caltech, and the “*MAGIC CPC*”, a self-sustaining, motion-tolerant, water-based condensation particle counter designed by Aerosol Dynamics Inc. The Magic Spider is compact, weighs 1.5 kg, and requires 12 Watts of power. It provides mobility-based particle sizing in the 10 – 500 nm range in as little as few seconds while operating on low flowrates (0.6 – 1.2 L/min sheath, and 0.3 L/min aerosol flow). It has been designed to provide sufficient statistics for atmospheric size distribution measurements in remote as well as urban locations.

Here, we present the key features of the integrated MAGIC Spider system, including determination of its transfer function over a range of sheath and aerosol flow rates. We examine both stepping and voltage-scanning operation, with scan times ranging from 90 s to as little as 1 s. The MAGIC Spider is compared against a benchtop Scanning Mobility Particle Sizer (SMPS) for both laboratory and ambient aerosols. The data show that particle size distributions agree well, as do the number concentration, geometric mean diameter and other integral parameters. The data further demonstrate the value of compositing fast scans over the benchtop’s two-min averaging period when examining rapidly changing aerosols.

6IM.5

On Passive Temperature Control and the Internal DMA Temperature in Hygroscopicity Tandem Differential Mobility Analyzers. CHRISTOPHER OXFORD, Brent Williams, *Washington University in St. Louis*

Two temperature control methods have been developed to limit the error in Hygroscopicity Tandem Differential Mobility Analyzers (H-TDMAs): active control and passive control (Swietlicki et al. 2008). In active control, H-TDMAs control both temperature and relative humidity in the second Differential Mobility Analyzer (DMA2). Since DMA2 and the measurement devices exist within the temperature-controlled volume, the measured relative humidity and temperature are equal to the relative humidity and temperature inside DMA2. In passive control, rules are used to distinguish accurate scans. These rules, based on measures of temperature and relative humidity, cull the results to achieve an acceptable error.

Active control has two error reduction advantages over passive control. Active control reduces temperature differences between DMA2 and the measurement devices and reduces temperature gradients within DMA2. In passive control, temperature gradients within DMA2 are present, and temperature/relative humidity differences between DMA2 and the measurement devices exist. Both active control benefits help increase the accuracy in H-TDMA measurements.

In this study, we placed a Resistance Temperature Device (RTD) inside DMA2 and measured the internal and external DMA2 temperature while measuring ammonium sulfate growth factors. The H-TDMA and the measurement devices were exposed to laboratory conditions, and heat transfer with laboratory air was encouraged using a box fan set to high. We compare the error due to the inference of DMA2 internal conditions with the remaining error (including DMA2 temperature gradients) to determine the primary benefit to active control. Additionally, we recommend new passive control rules for laboratory experiments.

6IM.6

Multi-Electrometer Detector for Real-Time High-Resolution Measurements in Planar Differential Mobility Analyzers. LUIS-JAVIER PEREZ-LORENZO, Mario Amo-Gonzalez, Juan Fernandez de la Mora, *Yale University*

Differential Mobility analyzers (DMAs) select a narrow range of particle mobilities in mixtures, determining mobility-distributions via voltage scans. To obtain high-resolution mobility spectra without scanning, we have distributed 100 electrically insulated charge-collecting strips over one electrode of a parallel plate DMA. All collected currents are sampled simultaneously, accelerating 100-fold the measurement. Initial tests with 8-detectors showed that suitably designed small steps in the insulating gaps between detectors do not induce turbulence. This development is particularly useful for high-resolution tandem DMA studies, typically requiring a grid of some 100x100 data points, and taking between 16.7 to 167 minutes. Incorporating the new detector into the second DMA makes the acquisition of tandem spectra as fast as current single spectrum acquisition (10-100 s), enabling a diversity of scientific investigations, such as the study of the evolution of small clusters. Another peculiarity of this DMA is that the usual finite sample flow rate at the outlet slit is null. The inlet sample flow rate can also be null in a parallel plate DMA, where charged particles may be injected by an external electric field. Therefore, the familiar inlet and outlet sample flow dependencies of the DMA size range and sensitivity no longer apply. Because the spectrum is obtained at fixed voltages, transmission corrections at the inlet and outlet are also simpler to implement than in scanning DMAs.

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6IM.7

Finding the Right Mass: Comparing Measurements from a Differential Mobility Analyzer, Aerodynamic Aerosol Classifier and Aerosol Particle Mass Analyzer. QI YAO, James Radney, Akua Asa-Awuku, Christopher Zangmeister, *National Institute of Standards and Technology*

There now exists an instrumentation trifecta for aerosol separation and classification by mobility diameter (D_m), aerodynamic diameter (as D_{aero} or the relaxation time, τ) and mass (m_p) utilizing a differential mobility analyzer (DMA), aerodynamic aerosol classifier (AAC) or aerosol particle mass analyzer (APM), respectively. In principle, any combination of two measurements yields the third; i.e. relaxation time = mobility \times mass. Here, we compare measurements of m_p , effective density and mass-mobility scaling exponents (D_{fm} , a surrogate for particle shape) utilizing different combinations of tandem measurements – DMA-APM, AAC-DMA and AAC-APM – utilizing ammonium sulfate, soot from a Santoro diffusion flame and water-soluble carbon black; notably, these particles represent a solid, near-spherical particle, a lacey aggregate and a near-spherical collapsed aggregate. Preliminary data suggests that deviations in m_p and D_{fm} between tandem measurements are low (on the order of 5 to 10 %) and that the largest uncertainty is the resolution of particles bearing multiple charges. While the AAC by itself does not require charge to classify particles, m_p (and hence D_{fm}) determination requires a secondary instrument (i.e. DMA or APM) that does separate based upon charge. Results show that the deconvolution of multiply charged particles with classical charging theory works well for the spherical particles (AS and carbon black) but is especially problematic for lacey soot. Thus, measuring particle mass from the AAC may have resolution limitations. We will also present recommendations for data analysis and interpretation.

6IM.8

Novel Approaches to DMA, CPMA, and APM Transfer Function Evaluation and Inversion to Determine Two-Dimensional Aerosol Mass-Mobility Distributions. TIMOTHY SIPKENS, Jason S. Olfert, Steven Rogak, *University of British Columbia*

Researchers are increasingly using tandem measurements of the mass and mobility to better characterize aerosols. Most commonly, this has involved using a differential mobility analyzer (DMA) in series with some kind of particle mass analyzer, such as the aerosol particle mass analyzer (APM) or centrifugal particle mass analyzer (CPMA). While most studies calculate some kind of summary parameter from this data, such as effective density or dynamic shape factor, more detailed information of the distribution of particle properties can be determined by instead determining the two-dimensional mass-mobility distribution. This presents unique challenges in terms of deconvolving the instrument functions, which mask the true distribution of properties. The present work expands on this problem in two significant ways. First, we consider novel approaches to evaluating APM and CPMA transfer functions, including particle tracking techniques that allow for closed-form expressions for these transfer functions under a wide range of flow and particle migration conditions. This has the capacity to greatly speed up the computations required to deconvolve tandem measurements. Second, we examine an array of inversion methods available to deconvolve the instrument functions to determine the two-dimensional mass-mobility distribution, including Tikhonov regularization, Twomey approaches, maximum entropy techniques (in the form of the multiplicative algebraic reconstruction technique or MART), and Bayesian or statistical approaches. This is to be demonstrated on simulated data and reveals that Bayesian approaches have the capacity to greatly improve reconstruction accuracy.

6RA.1

Revisiting Particle Dry Deposition: Observational Constraints of Submicron Aerosol and Black Carbon Fluxes. Delphine K. Farmer, ETHAN EMERSON, Holly DeBolt, Gavin McMeeking, Joshua P. Schwarz, Joseph Katich, *Colorado State University*

Dry deposition is a key process that removes particles from the atmosphere, and thus one factor that controls aerosol lifetime. Despite its importance, there are few measurements of particle dry deposition, and constraining model parameterizations has been challenging. Here, we use eddy covariance flux measurements of size-resolved sub-micron particle fluxes to investigate dry deposition over two terrestrial surfaces, including a ponderosa pine forest in Colorado and an agricultural site in Oklahoma. We contrast these observations with previous measurements in the literature, and with commonly used resistance models, highlighting several model-measurement discrepancies. To further investigate the mechanisms of dry deposition, we use black carbon deposition as an inert tracer for particle wet and dry deposition. We show that wet deposition dominates in the agricultural environment, and can provide observational constraints on black carbon lifetime in the region. Finally, size-resolved measurements of black carbon flux, with and without coatings, provides new insight into particle dry deposition mechanisms and our ability to capture this process with current models.

6RA.2

Aerosol Shape Classification by Deep Learning of Scattering Patterns. PATRICIO PIEDRA, Yong-Le Pan, Gordon Videen, *U.S. Army Research Laboratory*

Remote sensing of aerosol properties by inversion commonly requires directionally averaged aerosol light-scattering shape models such as spheres or spheroids. However, these shape-averaged models often yield discrepancies in retrievals at different wavelengths, leading to inaccurate or at-best ambiguous aerosol classification. Furthermore, shape-averaging does not allow discrimination of trace, non-averaged, scattering patterns. In this work, we have applied machine-learning algorithms to the calculated light-scattering patterns from particles of seven different, common, and naturally occurring shapes to test whether their shapes can be classified. Our scattering data set is produced from particles of volume-equivalent size parameter 5 and refractive index $m = 1.5 + 0i$, which have been isotropically and stochastically rotated. Furthermore, our dataset was either one-dimensional, depending on the polar angle, or two-dimensional, depending on both the polar and azimuthal angles. The neural network architectures required either a fully connected or a convolutional neural network. As expected, classification capabilities were much greater when the two-dimensional scattering data were used than when only one-dimensional data were considered. When the two-dimensional intensity patterns are considered, the prediction capabilities were approximately 70% for the regularly shaped particles and above 90% for the highly irregularly shaped particles. These capabilities increased slightly when linear polarization was used as input. These results suggest that high-accuracy (i.e., > 90 %) aerosol shape classification can potentially be achieved using a two-dimensional convolutional neural network.

6RA.3

Adsorption of VOCs by Airborne Dust Particles in the Semi-Arid Forest Canopy. BORIS KRASOVITOV, Andrew Fominykh, Itzhak Katra, Avi Levy, Andrey Khlystov, *Ben-Gurion University of the Negev, Israel*

Volatile organic compounds (VOCs) are naturally occurring chemicals that are highly volatile and thus found predominantly in the gas phase in the atmosphere. The mineral dust particles interact with VOCs emitted from a trees' leaves. Dust storms may significantly affect the concentration of VOCs in the atmosphere due to adsorption of VOCs by airborne dust particles. The developed model considers the interaction between the forest structure, open field and forest aerodynamics, aerosol and VOCs characteristics. Two-dimensional model is based on the application of theory of turbulent diffusion in the forest canopy in conjunction with models of VOCs release by leaves and gas adsorption by porous solid particles. The model of dust transport in the forest canopy is validated by comparison of theoretical results with measured dust concentrations. Measurements were conducted along a forest located in a semi-arid region (Northern Negev, Israel) to record PM concentrations in the forest and nearby environments during dust storms. The measurement results showed that during medium- and high-level dust storms, PM₁₀ concentrations in an urban environment that is located at the leeward side of the forest can be reduced by 28% compared with those of a nearby urban environment that is not affected by forest. Calculations performed using the developed model showed that despite a significant decrease in the PM concentration along the forest, dust particles can reduce the concentration of VOC by 7-10 % on the leeward side of the forest.

6RA.4

Chemical Composition of Individual Particles at a High-Altitude Mountain Station. KUO-PIN TSENG, Tyler Capek, Noopur Sharma, Angela Marinoni, Douglas Orsini, Claudio Mazzoleni, Swarup China, *Pacific Northwest National Laboratory*

The physicochemical properties of atmospheric particles play a critical role in cloud formation and their effects on climate. However, boundary layer and free tropospheric particles are different, and we have especially limited understanding of the physicochemical properties of free tropospheric aerosol. In this study, aerosol samples were collected from a high-altitude mountain site at Mt. Cimone, Italy, in July 2017. The site is representative of Southern Europe – Mediterranean background, but can also be affected by the plume from the Polluted Po Valley. The morphology and elemental composition of individual particles were analyzed via computer-controlled scanning electron microscopy and energy-dispersive X-ray spectroscopy. We also utilized other X-ray microspectroscopy to investigate the chemical bonding of individual particles. The results from different samples indicate that the particles had similar size distributions but different elemental composition. Back-trajectories suggest that emissions from the Mediterranean Sea, remote wildfires, and dust events contributed to the long-range transported aerosol at the site.

The sodium-rich particles, which likely originated from sea salts, constituted 29% of the collected aerosol in the morning, and dropped gradually to 8% in the afternoon. The back-trajectories and the elemental composition analysis suggest that the considerably low chloride in those particles is due to aging processes of sea salt transported from the Tyrrhenian Sea. Our analysis also show a large increase of carbonaceous particles, from 24% to 59%, at night. We observe the presence of tar balls in the night samples, as well. Unlike volatile organic particles, tar balls are stable under the electron beam. The increase of carbonaceous particles at night could be attributed to long range transport of biomass burning emissions. The morphological and chemical information on aerosol collected at high-altitude provides a better understanding of the atmospheric properties of free-tropospheric aerosol.

6RA.5

Impact of Seasonal Variabilities and Synoptic Conditions on Vertical Profiles of Trace Gas and Aerosol Properties over the Eastern North Atlantic. YANG WANG, Guangjie Zheng, Swarup China, Michel Jensen, Daniel Knopf, Alexander Laskin, Alyssa Matthews, David Mechem, Fan Mei, Ryan Moffet, Tamara Pinterich, Arthur J. Sedlacek, John Shilling, Stephen Springston, Jason Tomlinson, Daniel Veghte, Rob Wood, Maria Zawadowicz, Jian Wang, *Washington University in St. Louis*

Remote marine low cloud systems have large spatial and temporal coverages. Because of their relatively low optical thickness and background aerosol concentrations, marine low clouds are particularly susceptible to perturbations in aerosols associated with anthropogenic emissions. The response of low clouds to changes in atmospheric aerosols remains the major source of uncertainty in climate simulations. One major contribution to this large uncertainty derives from poor understanding of the marine aerosols under natural conditions, the perturbation by anthropogenic emissions, and the processes that drive them.

Here we present the vertical profiles of trace gases and marine aerosol properties and examine key aerosol processes using airborne measurements during the recent Aerosol and Cloud Experiments in the Eastern North Atlantic (ACE-ENA) field campaign. The Eastern North Atlantic (ENA) is a region of persistent but diverse subtropical marine boundary layer (MBL) clouds. During the ACE-ENA campaign, a total number of 39 research flights were conducted, 20 during summer 2017, and 19 during winter 2018. Gas species including water vapor, carbon monoxide, and ozone, and aerosol properties including number concentration, size distribution, optical properties, and chemical composition were measured onboard a Gulfstream-1 aircraft. Preliminary results show that the wintertime aerosol number concentrations were lower than those of summer both in the MBL and free troposphere (FT), and the Aitken mode aerosol in MBL often exhibits a smaller modal diameter during winter. These results suggest that a combination of fewer particles entrained from FT and slower condensation growth may contribute to the observed lower MBL cloud condensation nuclei concentration during winter, besides stronger coalescence scavenging by increased precipitation. The synoptic conditions during all flight days are classified into pre-front, post-front, and Azores high conditions. The properties and controlling processes of trace gases and aerosols in different seasons and under representative synoptic conditions will be discussed.

6RA.6

Rapid Chlorine Depletion in Nascent Sea Spray Aerosol by Condensed-Phase Aging Mechanisms. Noopur Sharma, SWARUP CHINA, Kuo-Pin Tseng, Daniel Knopf, Josephine Aller, *Pacific Northwest National Laboratory*

Sea spray aerosol (SSA) are produced at the sea surface by wave breaking and suspended into the marine boundary layer as a result of wind activity. In the atmosphere, these particles undergo multiphase chemical reactions leading to the depletion of their chloride ions, that have profound consequences on their physio-chemical properties. The aging process plays an important role in troposphere by contributing as a source of molecular chlorine in the atmosphere. As chlorine is depleted, particles undergo phase state and morphological transformations. Acidification of SSA by HNO_3 via displacement of the chlorine with nitrate ions is well established. Recently, it has been shown that organic acids, e.g. present as a coating of secondary organic aerosol, can also induce depletion of chlorine and the extent of reaction depends upon several factors like particle composition and acid strength, viscosity, mixing state, relative humidity, temperature and reaction time.

In this study, freshly generated nascent SSA samples collected during WACSII cruise from the western North Atlantic and Sargasso Sea in May 2014 onto substrates by impaction, were investigated for potential chlorine depletion and morphological changes. An array of micro-spectroscopy techniques: computer-controlled scanning electron microscopy coupled with energy dispersive X-ray microanalysis, scanning transmission X-ray microscopy with near-edge X-ray absorption fine structure analysis, and nano-secondary ion mass spectrometry were used to obtain the physio-chemical characteristics of individual particles. Our results indicate noticeable organic coating of the salt core and particles smaller than $1\mu\text{m}$ undergo considerable depletion of chlorine, despite their very brief exposure to ambient and humidified conditions. Here, we present the characterization of the chemistry at individual particle level, to improve the understanding of the aging process in sea salt particles and its characteristic timescales relevant for gas and particle chemistry in marine boundary layer.

6RA.7

Ammonium and Ammonia: Concentration Trends in the Northeast United States. JAMES SCHWAB, Hesham Hassan, Matthew Ninneman, Joseph P. Marto, Jie Zhang, Sara Lance, Christopher Lawrence, Fangqun Yu, Gan Luo, Arshad Nair, Kevin Civerolo, Oliver Rattigan, *University at Albany, SUNY*

Gas phase ammonia and its condensed phase counterparts – particulate ammonium and aqueous ammonium – comprise a critically important pool of reduced nitrogen compounds in the earth's atmosphere and biogeosphere as a whole. Ammonia is the most abundant base species in the atmosphere, playing critical roles in both aerosol nucleation and secondary aerosol growth, and providing a major nutrient input to terrestrial and aquatic ecosystems. For all these reasons it is important to understand changes in concentrations of both ammonia and ammonium; and the factors that influence their concentration trends. PM_{2.5} ammonium has been decreasing since around 2000, reflective of the similar trends in PM_{2.5} sulfate concentrations and sulfur dioxide emissions. While PM_{2.5} ammonium concentrations have been decreasing, gas phase ammonia concentrations have been increasing, an expected compensating effect given the largely stable NH₃ emissions reported by EPA inventories. Aqueous phase ammonium in precipitation and cloud water is more complicated, and recent data for the Northeast U.S. indicate it has been increasing over the past decade as well. These contrasting trends have produced a new regime in the aqueous phase charge balance in the Northeast U.S., with an ammonium cation surplus over the combined nitrate and sulfate anion strength emerging as the typical condition of cloud and rain water in the past couple years. This presentation will explore these trends, the factors contributing to them, and their implications for aerosol formation, atmospheric chemistry, and ecosystem response.

6RA.8

Influence of Agricultural Emissions and the Chesapeake Bay on Urban Aerosol Chemistry in Baltimore, Maryland. MICHAEL BATTAGLIA JR., Nicholas Balasus, Kat Ball, Ruben Delgado, Christopher Hennigan, *University of Maryland, Baltimore County*

As part of the NASA OWLETS-2 field campaign, we characterized aerosol composition and gas-phase ammonia concentrations at an urban land-water transition site located in the upper Chesapeake Bay. Several intense pollution episodes were captured throughout the course of the campaign, with daytime aerosol nitrate concentrations much higher ($> 5 \mu\text{g m}^{-3}$) than is typically observed in the eastern U.S. during summer. The ISORROPIA-II aerosol thermodynamic equilibrium model was utilized to compute aerosol pH, aerosol liquid water (ALW) and ammonia gas-particle partitioning. These predictions were paired with HYSPLIT back trajectory modeling predictions to identify source origin and transport times during these periods. The results indicate significant ammonia contributions from poultry farms on Maryland's Eastern Shore and dairy farms in southeastern Pennsylvania. Ammonia concentrations showed a distinct diurnal profile but were consistently high throughout the study (mean $\sim 4 \mu\text{g m}^{-3}$), suggesting the importance of emissions from both agricultural regions. The HU-Beltsville CASTNET site was used as inland site for comparison of the observed trends. These results are likely to have broad implications on aerosol chemistry in regions with diverse and meteorologically-driven changes in source influences, as well as for pollution control strategies in coastal urban areas.

6SA.1

A Global Modeling Source Apportionment of PM_{2.5}: Identifying Major Sources and Quantifying Sensitivities to Policy Relevant Reductions. ERIN MCDUFFIE, Melanie Hammer, Michael Brauer, Steven Smith, Randall V. Martin, *Dalhousie University, Halifax, Canada*

Fine particulate matter (PM_{2.5}) is the leading environmental risk factor for human health, attributable to an estimated 5.2% of all deaths in 2017. To reduce ambient PM_{2.5} exposure, contributions from major emission sectors must be quantified. An increasing number of source attribution studies have utilized 3D chemical transport models due to their ability to assess contributions at continental or global scales. Much of this recent work has been conducted at regional/country scales, with emissions divided into coarse emission sectors (Transportation, Industry, Energy, etc.). While some studies have investigated global-scale contributions, these aggregate sectoral contributions are primarily quantified using a 'zeroing-out' method where entire sectors are removed and compared to base simulations. Removal of large, aggregate sectors can result in a nonlinear response of PM_{2.5} due to changes in the chemical limitations of secondary aerosol production. Such nonlinear effects are recognized, but not well quantified, leading to a potential bias in estimated sectoral contributions and associated health burden of PM_{2.5}. There is increasing interest in investigating global PM_{2.5} sources at finer sectoral resolution and for evaluating policy-relevant reductions (~10-50%), thereby reducing the nonlinearities of previous methods.

This work presents global simulations from the GEOS-Chem model (v12) to quantify nonlinear emission contributions to annual PM_{2.5} mass. The work leverages the recently-developed Community Emissions Data System (CEDS) to investigate individual contributions from heating, cooking, and coal and biomass combustion from residential energy use, coal combustion from industrial and energy sectors, shipping, aircraft, on-road, and non-road/rail emissions from the transportation sector, as well as emissions from agricultural activities, open fires, solvents, biogenic sources, and dust. Additional simulations of policy-relevant reductions highlight the chemical sensitivities of PM_{2.5} under current emission scenarios and evaluate nonlinearities of previous methods, providing a framework for future studies.

6SA.2

Extensive Source Apportionment of PM_{2.5} Organic Aerosols in New Delhi. ANNA K. TOBLER, Deepika Bhattu, Francesco Canonaco, Sachchida N. Tripathi, Suresh Tiwari, Jay G. Slowik, Urs Baltensperger, Andre S.H. Prévôt, *Paul Scherrer Institute*

Because atmospheric aerosols are recognized to have adverse effects on climate, visibility and human health, the identification and source apportionment on those particles is of great importance. In 2018, New Delhi was ranked the most polluted capital in the world regarding PM_{2.5} mass concentrations. To study the long-term PM_{2.5} mass concentration and its chemical composition evolution in New Delhi, an Aerodyne Time-of-Flight Aerosol Chemical Speciation Monitor (ToF-ACSM) was installed at the Indian Institute of Tropical Meteorology (IITM) for over a year.

In this study, we present the high time-resolved, detailed chemical composition of non-refractory PM_{2.5} in New Delhi. In the winter season, total non-refractory peak concentrations over 400 µg/m³ and chloride concentrations exceeding 100 µg/m³ were routinely observed, whereas the concentrations in summer are much lower. The complex organic mass spectra were further analyzed with positive matrix factorization (PMF) within the Source Finder (SoFi) software. Two primary factors, hydrocarbon-like organic aerosol (HOA) and solid fuel combustion organic aerosol (SFC-OA), were resolved besides the more oxygenated organic aerosol factors. The PMF results suggest that chloride could play an important role in the oxidation processes. To overcome the limitation of the assumption of constant sources within the PMF algorithm, a small and rolling PMF window is moved over the dataset to allow the factor profiles to vary over time. In addition, to estimate the statistical uncertainty of the PMF solution, PMF runs were resampled using the bootstrap algorithm.

6SA.3**Wintertime PM_{2.5} 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, Robert J. Yokelson, Peter DeCarlo, Elizabeth Stone, *University of Iowa*

Wintertime particulate matter composition and sources were examined in the Indo-Gangetic Plain (IGP) and Kathmandu Valley during the second Nepal Ambient Monitoring and Source Testing Experiment (NAMaSTE 2) from December 2017-February 2018. In Lumbini, located in the northern IGP, daily average PM_{2.5} and PM₁₀ concentrations ranged 48-295 $\mu\text{g}/\text{m}^3$ and 60-343 $\mu\text{g}/\text{m}^3$, respectively, with organic carbon (OC) comprising 45% of PM_{2.5}. By way of molecular markers, biomass burning, cow dung burning, and garbage burning were identified as major PM_{2.5} sources. Nitro-monoaromatic compounds, of interest due to their light-absorbing properties and toxicity were measured for the first time in the region. Three such species, 4-nitrocatechol (2-434 ng/m^3), 4-methyl-5-nitrocatechol (0.1-201 ng/m^3), and 5-nitrosalicylic acid (8-61 ng/m^3) indicated the presence of secondary organic aerosol (SOA) associated with biomass burning. Additional SOA precursors included anthropogenic monoaromatic and diaromatic volatile organic compounds (VOCs) that had consistently larger SOA contributions than isoprene, monoterpenes, and sesquiterpenes. In Kathmandu, Lalitpur, and Dhulikhel in the Kathmandu Valley, PM_{2.5} and PM₁₀ concentrations ranged 31-183 $\mu\text{g}/\text{m}^3$, and 57-433 $\mu\text{g}/\text{m}^3$, respectively, of which OC comprised 28-31%. Garbage burning, fossil fuel combustion, and biomass burning were identified as major PM_{2.5} sources. In comparison to Lumbini, the Kathmandu Valley had larger influences from garbage burning and fossil fuel sources and substantially lower influences from dung burning. Trends in SOA precursors were consistent across the Kathmandu Valley and IGP, with larger influences from anthropogenic VOCs compared to biogenic VOCs. Chemical mass balance modeling will be used for source apportionment to estimate source contributions to PM_{2.5} organic carbon during pollution events.

6SA.4**Characterization of Black Carbon and Trace Metals Using Soot-Particle Aerosol Mass Spectrometer: Insight into Organic Aerosol Sources in a Complex Urban Environment.**

LAURA-HELENA RIVELLINI, Max Adam, Nethmi Kasthuriarachchi, Alex Lee, *National University of Singapore*

Atmospheric carbonaceous aerosol have significant impacts on human health and climate. Understanding how emissions and atmospheric processes can influence their physico-chemical properties is essential to evaluate such impacts. Co-emission of black carbon (BC) and primary organic aerosol (POA) from combustion and secondary OA (SOA) formation on BC through oxidation of gas-phase precursors and POA are well-known. However, the relative importance of individual BC source and how BC interact with OA during chemical aging remains largely unexplored.

A soot-particle aerosol mass spectrometer (SP-AMS) was deployed to characterize OA, refractory BC (rBC) and trace metals in Singapore, a highly urbanised city in the Southeast Asia. In addition to OA fragments, rBC and trace metals ions were integrated to our positive matrix factorization for source apportionment analysis. This work provides evidence that fuel combustion-related OA (hydrocarbon-like OA) and less-oxidised oxygenated OA (LO-OOA, i.e., fresh SOA produced via photochemistry under the influences of industrial emissions) are largely associated with rBC (63 and 29% respectively). In contrast, cooking-related OA (COA) and more-oxidised OOA (MO-OOA, i.e., more aged OA) factors were composed of low rBC content (<10% of total rBC). Potassium and rubidium were mainly associated with MO-OOA, indicating the significance of biomass burning emissions from the nearby countries to this aged OA component.

Furthermore, C_1^+/C_3^+ and V/Ni ratios are used to identify different types of combustion. In particular, the aerosol pollutants transported from industrial area and shipping ports gave higher C_1^+/C_3^+ (~ 1.0) and V/Ni ratios than those associated with traffic ($C_1^+/C_3^+ < 0.8$). Single particle measurements will be discussed to evaluate the aerosol mixing state emitted from the identified sources. Overall, this work demonstrates that the rBC fragments and trace metal characterized by SP-AMS can provide important insight into the sources and characteristics of OA in a complex urban environment.

6SA.5

Developing a Four-dimensional Variational Assimilation Framework for Refining U.S. Ammonia Emissions with Size-Resolved Aerosol. SHANNON CAPPS, Mahmoudreza Momeni, Matthew Lombardo, Amir Hakami, Daven Henze, Steven Thomas, Jeremy Silver, Peter Rayner, CMAQ Adjoint Development Team, *Drexel University*

Chemical transport models such as the Community Multiscale Air Quality (CMAQ) model provide a platform for evaluating the influence of emissions on atmospheric composition. They are designed to represent scientific consensus on the chemical and physical transformations of emitted species into pollutant concentrations. For processes represented with sufficient certainty, such as transport, aerosol dynamics, and inorganic aerosol thermodynamics, the difference in modeled and observed concentrations is useful for evaluating the emissions inventory. Specifically, these differences in concentration can be leveraged in a four-dimensional variational assimilation framework to provide revised estimates of emissions with spatial specificity.

This work introduces the CMAQ adjoint integrated in a Python-based four-dimensional variational framework. Given the difficulty of estimating emissions of ammonia from the agricultural sector and the complexity of relating emissions to concentrations of this condensable species, this work focuses on the refinement of ammonia emissions through satellite observations of ammonia from the Cross-track Infrared Sounder (CrIS). The assimilation of CrIS pseudo-observations demonstrates the capability of the framework to improve estimates of perturbed emissions.

6SA.6

Excitation-Emission Matrix Fluorescence Spectroscopy for Source Apportionment of Combustion Sources: Comparison to Positive Matrix Factorization Results from an Exposure Assessment Panel Study. JAY RUTHERFORD, Timothy Larson, Edmund Seto, Igor Novosselov, Jonathan Posner, *University of Washington*

Although many consider the link between particulate matter (PM) and negative health effects as a well-established fact, the significance and estimated severity of these health effects have been a topic of recent debate. To address these ongoing questions and to help inform effective mitigation strategies into the future, further study of PM health effects is necessary. The development of low-cost particle counters has enabled highly resolved spatial and personal measurement of PM, but these devices don't allow for source apportionment.

Here we present a method for identifying PM source using excitation-emission matrix (EEM) fluorescence spectroscopy and machine learning algorithms aimed at enabling low-cost PM source apportionment. Previously we presented an EEM-machine learning method to identify combustion generated PM_{2.5} from wood smoke, diesel soot, and cigarette smoke from personal exposure monitoring filters collected in a laboratory environment. In the present work, we apply the same EEM-machine learning methodology to identify combustion sources present in PM samples collected during an exposure assessment panel study. We obtained archived field samples from the panel study and the associated positive matrix factorization (PMF) source apportionment results that used elemental analysis by X-ray fluorescence and light absorbing carbon measurements. We show that EEM spectra from cyclohexane extracts of these filter samples can be used to predict the same combustion sources determined by PMF with R² values up to 0.84. The use of this EEM-machine learning approach may be used to conduct PM exposure studies that include source apportionment of combustion sources at a low-cost.

6SA.7

Emissions from Rural and Urban Open Waste Burning in Ghana. DAVID PFOTENHAUER, Evan Coffey, Ali Moro, Maxwell Dalaba, Abraham Oduro, Jeremiah Asumbere, John Nyante, Maxwell Sunu, Emmanuel Appoh, Michael Hannigan, *University of Colorado, Boulder*

In many nations, citizens burn waste as the only method for its removal. The emissions from open waste burning are still poorly understood, and their contribution to ambient pollution and human exposure unexplored. We collected gaseous and particle phase emission data from many rural and urban trash burning events in Ghana. We sorted and weighed select trash piles prior to burning to estimate typical composition and weight distributions. Emission factors for gaseous pollutants, carbon monoxide (CO) and carbon dioxide (CO₂), as well as particulate matter (PM) were calculated for each trash burning event. We further analyze the samples for organic species using gas chromatography mass spectrometry (GCMS) methods and confirm molecular tracers that can be used to assess waste burning source contributions to ambient pollution. Finally, we isolate and measure emissions from specific plastic types and waste composites to determine material contributions to bulk waste burning emissions.

6SA.8

Impact of Emissions from Incomplete Combustion Sources, Biomass Burning and Fossil Fuel, on Ambient Concentrations of Black Carbon (BC) in the Milan Metropolitan Area. AMIRHOSEIN MOUSAVI, Mohammad Sowlat, Christopher Lovett, Martin Rauber, Soenke Szidat, Roberto Boffi, Alessandro Borgini, Cinzia De Marco, Ario Ruprecht, Constantinos Sioutas, *University of Southern California*

In the current work, spatial and temporal variation of black carbon (BC) concentrations originated from two important combustion sources, i.e. fossil fuel combustion and biomass burning, were evaluated at two sites, including Milan, a metropolitan area primarily impacted by urban emissions, and Bareggio, a sub-urban area located 14 km to the west of Milan, from summer 2017 to winter 2018. Using the Aethalometer model, sources of BC were apportioned based on the measurements performed using seven-wavelength (AEE33) and single-wavelength (AEE51) Aethalometers in Milan and Bareggio sampling sites, respectively. Our measurements demonstrated higher average combustion-generated BC concentrations at the Bareggio site ($2763 \pm 1050 \text{ ng.m}^{-3}$) in comparison to the Milan site ($1921 \pm 876 \text{ ng.m}^{-3}$). The Aethalometer model suggested a slightly higher annual average contribution of BC originated from fossil-fuel combustion (%BCff) in Milan ($84.9 \pm 5.4\%$) than in Bareggio ($\pm 4.1\%$); however, contributions from biomass burning originated BC (%BCbb) were considerably higher in Bareggio (e.g., a wintertime average of $61.3 \pm 5.3\%$) than in Milan (e.g., a wintertime average of $30.5 \pm 4.6\%$). Furthermore, %BCff trends showed a peak during the morning and afternoon rush hours in both Milan and Bareggio, when the highest traffic activities are expected. On the other hand, a nighttime peak was observed for %BCbb when emissions from residential wood burning for heating purposes was prominent. In spite of the fact that traffic is a major source of combustion generated BC particles in the metropolitan Milan, our findings also revealed the key role of emissions from the residential wood burning on ambient BC concentrations in the area.

7AC.1

Condensed Phase Photochemical Reactions of Secondary Organic Aerosols: Photodegradation & Photosensitized Reactions. VAHE BABOOMIAN, Xinke Wang, Rachel Gemayel, Yiran Gu, Lisa M. Wingen, Chrisitan George, Dmitry Fishman, Sergey Nizkorodov, *University of California, Irvine*

The sunlight driven transformations of atmospheric organic aerosols are important for understanding and controlling the climate and health-relevant properties of particulate matter, but these photochemical processes are not well understood. Molecules within aerosol particles are often considered shielded from reactions with oxidants but this view does not include condensed phase photochemical reactions. Our report presents experimental studies identifying the long-term physical and compositional changes occurred due to photochemical aging as well as the mechanisms responsible for them. The physical changes were investigated by utilizing a quartz crystal microbalance to quantify the mass loss rate from various lab generated particles irradiated at various wavelengths. We observed that 254 nm irradiation degraded 86 % of toluene secondary organic aerosol (SOA) after 24 hours, but only 74 % of α -pinene SOA suggesting different levels of resilience. The compositional changes due to long term irradiation were also investigated using High Resolution Mass Spectrometry techniques. The chemical mechanisms responsible for this aging include direct photochemical processes, such as Norrish type splitting of carbonyls, as well as indirect photosensitized reactions. Photosensitized reactions involve energy transfer from an initial chromophore (photosensitizer/ $^3C^*$) to a neighboring molecule which creates a cascade of chemical reactions that may drastically alter the chemical composition of the particle. These reactions were investigated by probing the triplet states of naphthalene SOA on ultrafast femtosecond and nanosecond timescales. Ultrafast experiments clearly demonstrate triplet states being populated within a few picoseconds and decay with a lifetime of a few microseconds. This unexplored aging mechanism shows that even photostable molecules within aerosols can undergo reactive energy transfer without directly absorbing sunlight, thus elucidating a new channel of photochemical aging.

7AC.2

Impact of Photochemical Aging on SOA Yield and Equilibrium Partitioning Predictions. JOHN SHILLING, Maria Zawadowicz, Jiumeng Liu, Rahul Zaveri, Alla Zelenyuk, *Pacific Northwest National Laboratory*

Organic aerosol is the largest fraction of the atmospheric non-refractory aerosol mass and has a significant impact on climate, visibility, and human health. A significant portion of organic aerosol is secondary organic aerosol (SOA), which forms when volatile organic compounds (VOCs) are oxidized and the reaction products partition to the particle phase. SOA formation and aging have been described using semi-volatile partitioning theory, and a typical assumption invoked is that gas-particle partitioning rapidly reaches equilibrium. However, several studies have called into question whether traditional equilibrium assumptions are valid, either due to particle-phase diffusion limitations, particle-phase reactions, or liquid/liquid phase separation and immiscibility of organic phases. Here, we investigate the ability of partitioning theory to describe laboratory SOA formation experiments using SOA mass yield as the evaluation metric. We conduct two types of experiments; co-condensation experiments in which isoprene and α -pinene are simultaneously oxidized to form SOA, and sequential condensation experiments in which fresh isoprene SOA is exposed to aged, pre-existing isoprene and α -pinene particles. In the co-condensation experiments, partitioning theory successfully predicted the time-dependent SOA concentrations without invoking diffusion limitations or organic phase separation. However, in the sequential condensation experiments, yield analysis showed that fresh isoprene SOA did not partition into either the aged α -pinene or isoprene SOA particles on the experimental timescale, even at relative humidity as high as 85%. This study shows that common assumptions regarding SOA gas-particle partitioning are accurate for fresh SOA, but that these assumptions break down after SOA has been photochemically aged for modest amounts of time (~ 1 day). These results have important consequences for modeling SOA formation and may help to resolve some seemingly divergent conclusions regarding diffusion limitations that exist in the literature.

7AC.3

Photodegradation of Alpha-pinene Secondary Organic Aerosol. Veronika Pospisilova, DAVID BELL, Imad El Haddad, Lamkaddam Houssni, Amelie Bertrand, Josef Dommen, Andre S.H. Prévôt, Urs Baltensperger, Jay G. Slowik, *Paul Scherrer Institute*

Secondary organic aerosol (SOA) species create a large fraction of atmospheric aerosol mass. These particle-phase organics can be affected by various processes such as evaporation, particle-phase reactions or photochemical aging, leading to a change of particle properties. Small organic molecules, likely products of photodegradation, have been identified in the gas phase upon SOA irradiation and decrease in organic mass together with changes in the bulk chemical composition upon UV light exposure was reported. However, little is known about the effect of UV radiation on the chemistry of oxidized SOA species as direct molecular level observation of condensed-phase organics and the associated changes in the physico-chemical properties (e.g. volatility) are lacking. Therefore, the particle-phase photochemical changes are likely underestimated.

To investigate the effect of solar radiation on the molecular composition of SOA formed from α -pinene ozonolysis we performed a series of experiments simulating the photochemistry using a set of 40 UV lights (90–100 W) and measuring the particle-phase composition with an extractive electrospray time-of-flight mass spectrometer (EESI-TOF). EESI-TOF provides real time measurement of aerosol species unaffected by thermal decomposition or ionization-induced fragmentation. All experiments were performed in batch-mode in Teflon chamber with 40-50% relative humidity. In addition, isothermal evaporation measurements were conducted of SOA before and after UV lights.

We show that the behavior of individual α -pinene SOA species in the particle phase is altered upon the UV irradiation. We observe significant decay of certain molecules after the UV lights are turned on dependent on the particle mass loading and presence of isomers of different photo-stability. We determined the particle-phase photolytical rates to be on the order of $0.5 - 2 \cdot 10^{-3} \text{ s}^{-1}$ on average, corresponding to lifetimes of $\sim 8\text{-}30\text{min}$. Further, significant decrease in the effective volatility of photochemical aged SOA is observed.

7AC.4

Ozonolysis of Polycyclic Aromatic Hydrocarbons on the Surfaces of Secondary Organic Aerosol Particles. ALLA ZELENYUK, Kaitlyn J. Suski, David Bell, Dan Imre, Simeon Schum, Lynn Mazzoleni, ManishKumar Shrivastava, Amber Kramer, Staci L. Simonich, *Pacific Northwest National Laboratory*

Polycyclic aromatic hydrocarbons (PAHs) are toxic pollutants emitted as byproducts of energy production and consumption that can undergo long-range transport into remote regions of the world. We have previously shown that the presence of gas-phase PAHs during secondary organic aerosol (SOA) formation significantly affects particles mass loadings, composition, growth, volatility, and viscosity. Compared to “pure” SOA, these particles have higher viscosity and higher fraction of non-volatile compounds, i.e. oligomers. These particles also contain unreacted PAHs and products of heterogeneous reactions between PAHs and ozone that are trapped within the bulk of the highly viscous SOA, shielded from evaporation and oxidation. Here we will present detailed analysis of particle composition using real-time single particle mass spectrometry, bulk aerosol mass spectrometry, and offline analysis of the aerosol extracts using gas chromatography–mass spectrometry and ultrahigh resolution Orbitrap Elite mass spectrometry with four complementary ionization techniques. We will discuss the chemical mechanisms responsible for increased SOA formation yields and formation of oligomers.

Furthermore, we will show that heterogeneous ozonolysis of PAHs on the surfaces of “pure” biogenic SOA particles results in the formation of shells composed of oxidized PAHs and trapped unreacted PAHs, which alter particles volatility. The formation of shells was quantified by measuring changes in particle size and composition. The volatility of these particles was lower than that of “pure” α -pinene SOA, and most notably, a significant fraction of the PAHs and their oxidation products remained in the particles after a day of evaporation under dry or high RH conditions.

These results suggest that PAHs can become incorporated into SOA particles at any time during their atmospheric lifecycle via adsorption and surface reactions with ozone. These reactions affect the composition, morphology, and evaporation kinetics of these particles and can lead to longer than traditionally predicted atmospheric lifetimes of PAHs.

7AC.5

Compositional Evolution of Secondary Organic Aerosol as Temperature Cycles in Atmospherically Relevant Ranges.

Zixu Zhao, Chen Le, Qi Xu, Weihang Peng, Huanhuan Jiang, Ying-Hsuan Lin, David R. Cocker III, HAOFEI ZHANG, *University of California, Riverside*

Atmospheric secondary organic aerosols (SOA) play an important role in the global particulate matter budget, and their chemical compositions determine critical properties that impact radiative forcing and human health. During atmospheric particles' temporal and spatial transport, they could undergo ambient temperature change or cycle through various mechanisms that may transform their chemical compositions. Here, we report the compositional evolution of SOA from α -pinene ozonolysis in a smog chamber as the temperature cycles within atmospherically relevant ranges. Combining a number of on-line and off-line aerosol bulk and molecular-level measurements, we conclude that: (1) as the temperature drops, the organic vapor condensation is much less pronounced compared to volatility-based predictions, likely due to the high viscosity of the α -pinene SOA particles; (2) active and complex particle-phase reactions occur reversibly and irreversibly throughout the temperature cycles, substantially modifying concentrations of the SOA constituents and forming new products; and (3) the SOA bulk O:C ratios increase steadily during most temperature cycles in the absence of gas-phase hydroxyl radicals, and we propose a particle-phase isomerization mechanism of alkoxy radicals from organic peroxide decomposition to account for the observations. These findings have important implications for understanding the chemical evolution of SOA in the atmosphere through their lifetime and long-range transport.

7AC.6

Chemical Transformation of Isoprene Epoxydiol-Derived Organosulfates through Heterogeneous OH Oxidation: A Source of Inorganic Sulfate?

Hoi Ki Lam, Kai Chung Kwong, Hon Yin Poon, James F. Davies, Zhenfa Zhang, Avram Gold, Jason Surratt, MAN NIN CHAN, *The Chinese University of Hong Kong*

Multiphase chemistry of epoxydiols formed from isoprene oxidation yields the most abundant organosulfates (i.e., methyltetrol sulfates) detected in atmospheric fine aerosols. This potentially determines the physicochemical properties of fine aerosols in isoprene-rich regions. To date, the transformation of these organosulfates in the atmosphere remains largely unclear. We investigate the heterogeneous oxidation of aerosols consisting of potassium 3-methyltetrol sulfate ester ($C_5H_{11}SO_7K$) by gas-phase hydroxyl radical (OH) through studying the oxidation kinetics and reaction products at a relative humidity (RH) of 70.8%. Real-time molecular composition of the aerosols is obtained by using a Direct Analysis in Real Time (DART) ionization source coupled to a high-resolution mass spectrometer. Aerosol mass spectra only show increases in the intensity of bisulfate ion (HSO_4^-) after oxidation, suggesting the absence of functionalization processes that is likely attributable to the steric effect of substituted functional groups (e.g. methyl, alcohol and sulfate groups) on peroxy-peroxy radical reactions. Overall, potassium 3-methyltetrol sulfate ester likely decomposes to form volatile fragmentation products and aerosol-phase sulfate radical anion ($SO_4^{\bullet-}$). $SO_4^{\bullet-}$ subsequently undergoes intermolecular hydrogen abstraction to form HSO_4^- . Given the high atmospheric abundance of organosulfates in atmospheric aerosols, further study of the contribution and transformation of organosulfates to inorganic sulfate through chemical reactions (e.g. heterogeneous oxidation, aqueous-phase oxidation and hydrolysis) is desirable.

7BC.1

Long-range Transported North American Wildfire Aerosols Observed in Marine Boundary Layer of Eastern North Atlantic. Guangjie Zheng, Arthur J. Sedlacek, Allison Aiken, Yan Feng, Thomas Watson, Shira Raveh-Rubin, Janek Uin, Ernie R. Lewis, JIAN WANG, *Washington University in St. Louis*

Biomass burning aerosols greatly impact climate by interacting with solar radiation and clouds, and wildfires are major sources of biomass burning aerosols. Compared to tropical grassland or Eurasia boreal forests, tree species in North America (NA) boreal forests can support high-intensity crown fires. The resulting stronger pyrocumulonimbus activities can inject NA wildfire aerosols to higher altitudes, where they can exert a stronger influence on Earth's radiation balance and be spread over larger geographic areas. Moreover, frequency and intensity of NA wildfires have been greatly enhanced by global warming in recent decades, and are expected to further increase in the future.

Properties of aerosols from NA wildfires may vary substantially during their transport in the atmosphere, but this variation would be missed by most previous studies that were conducted in near-field. Here we present comprehensive characterization of climatically relevant properties of aged NA wildfire aerosols emitted from the record-breaking Canadian wildfires in August 2017. Despite the elevated injection height (13~20 km), these aerosols were transported downward into the marine boundary layer of eastern North Atlantic over a period of 10 days, owing to the dry intrusions in mid-latitude cyclones. The aged wildfire aerosols exhibited elevated single scattering albedos (0.93 to 0.96) at 529 nm, and low absorption Ångström exponents of less than 1 for 464 nm/648 nm pair, suggesting negligible brown carbon contribution and thick coatings. The hygroscopicity parameter, κ , ranged 0.2 to 0.4. Both aerosol size distribution and κ of the aged wildfire aerosol are similar with those previously reported in fresher wildfire plumes in NA free troposphere, suggesting minor changes in overall CCN activity during the long-range transport in free troposphere. However, the CCN activities differ substantially from those typically assumed in global climate models and those observed in south Africa, highlighting the need for more detailed model representation.

7BC.2

Western US Wildfire Emissions of Ice Nucleating Particles. PAUL DEMOTT, Kevin Barry, Ezra Levin, Kathryn Moore, Thomas Hill, Cynthia Twohy, Darin Toohey, Amy P. Sullivan, Sonia Kreidenweis, Emily Fischer, *Colorado State University*

The sources, abundance and nature of emissions of ice nucleating particles (INPs) affect aerosol-cloud interactions, precipitation, and climate in ways that are not well characterized. Contribution of biomass burning INPs is particularly poorly resolved. Most previous sampling of INPs emitted during wildfires was conducted from surface sites. There is need to examine INP emissions directly in wildfire plumes, including subsequent interactions with clouds, as INP inputs may vary with fire size, fuel, combustion efficiency and age, and may include lofted soils, ash, and plant material [McCluskey et al., *J. Geophys. Res. Atmos.*, 119, 10,458–10,470, 2014].

INP measurements using an online continuous flow diffusion chamber and bulk offline filter collections for immersion freezing measurements were made via an isokinetic inlet, and from smoke-affected cloud particle residues via a counterflow virtual impactor inlet on the NSF/NCAR C-130 as part of the Western Wildfire Experiment for Cloud Chemistry, Aerosol, Absorption and Nitrogen study. Based from Boise, ID in summer 2018, numerous plumes and diffuse smoke regions were sampled over the intermountain west and northwest United States. In agreement with previous surface-based studies, order of magnitude average enhancements in INPs were observed in wildfire plumes compared to background air, indicating highly selective production of INPs compared to greater enhancements of total particles. Production with aging was inferred in some cases.

INP compositions, determined by TEM/EDS and chemical treatments of bulk samples, were dominated by thermally stable organic carbon mixtures with sulfates and other inorganics. Mineral and mixed INPs were always found, although in the minority compared to organic types. INP mode size was below 500 nm in cases analyzed thus far. Future work will develop parameterizations for wildfire INP sources over the full mixed-phase cloud temperature range, and utilize these for numerical modeling studies.

7BC.3

Latitudinal Shifts in Wildfire Activity and Smoke Concentrations in Response to 21st Century Climate and Land Cover Change over the Western US. YANG LI, Loretta Mickley, Jed Kaplan, Pengfei Liu, *Harvard University*

Recent studies have projected increasing trends of wildfire activity under a warmer and drier climate in the western US, with implications for air quality due to increasing smoke particulate matter (PM). However, there exists large uncertainty in these projections, and not all studies have taken changing land cover or land use into account. Here we implement a coupled modeling approach to assess the impacts of future changes in climate and land use/ land cover on wildfires, and to investigate the consequences for surface air quality. We rely on a process-based fire model linked to a dynamic global vegetation model (LPJ-LMfire) and a global chemical transport model (GEOS-Chem) to examine smoke trends across the 21st century for different Representative Concentration Pathways (RCPs) in the western US. Under a scenario of moderate climate change (Representative Concentration Pathway 4.5, or RCP4.5), we find that increasing fire activity in the western US enhances the burden of smoke fine particulate matter (PM_{2.5}) across the West, with increases of ~54% by the late-21st century during the fire season (July-September). In the worst-case scenario (RCP8.5), smoke PM_{2.5} concentrations across the West nearly double by 2100 during the fire season. RCP8.5 also shows large, northward shifts in living biomass and thus dry matter burned, leading to especially increased fire activity in northern states, such as Montana and Wyoming. Regions east of the Rocky Mountains also experience enhanced fire activity.

7BC.4

The Sources and Evolution of Ice Nucleation Particles Emitted by Biomass Burning. LYDIA JAHL, Leif Jahn, Michael Polen, Thomas Brubaker, Bailey Bowers, Sara Graves, Ryan Sullivan, *Carnegie Mellon University*

Surprisingly, the combustion of some biomass fuels has been found to produce ice nucleating particles (INPs) that induce immersion freezing at temperatures as warm as -20 °C. Biomass burning thus represents a potentially large but unconstrained source of INPs to the atmosphere that can significantly change cloud microphysics, precipitation, and climate. The source of these ice nucleating particles (INPs) is still under investigation; soot particles do not appear to account for all INPs emitted by biomass burning. We report measurements of efficient INPs in the bottom ash and aerosol produced from biomass burning. The ash from tall grass fuels that combust intensely were found to contain a larger fraction of crystalline material through X-ray diffraction analysis, which likely explains the higher ice activity of the ash. The biomass burning aerosol from these fuels also contained efficient INPs. Biomass burning can therefore introduce new ice-active mineral phases produced by combustion into the atmosphere, in addition to lofting pre-existing mineral and soil particles that may also act as INPs. Fuels that contain higher mass fractions of elements such as calcium and silicon tend to produce more crystalline content upon combustion, providing a connection between the original fuel and the new mineral phases formed in the aerosol and ash, and their ice nucleation activity.

Biomass burning aerosol undergoes extensive physical and chemical transformations during atmospheric transport, and we examined how this evolution might alter the ice nucleation properties of the aerosol. The chemical aging of combustion aerosol from a variety of biomass fuels including sawgrass, birch, cutgrass, and black needlerush was simulated using a smog chamber reactor. Aging such as through dark ozonolysis or UV photolysis of HONO, was often found to enhance the ice activity of the aerosol. We hypothesize that aging makes the mineral-based ice nucleants more accessible to water and thus ice crystal formation. The chemical composition of the aerosol prior to and following aging 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. Our novel microfluidic droplet freezing assay allowed us to reliably determine the immersion freezing temperature of the aerosol down to -32 °C, critically enabling measurements at lower temperatures where biomass burning aerosol typically induces freezing. We will present our findings on the changes in the aerosol's composition following chemical aging, and how this correlates with the ice nucleating abilities of fresh and aged biomass burning emissions.

7BC.5

Significant Impact of Transported African Biomass Burning on Phosphorus Deposition and Biogeochemical Cycles in the Amazon and Tropical Atlantic Ocean. Anne Barkley, Joseph M. Prospero, Natalie Mahowald, Douglas Hamilton, Kimberly Popen Dorf, Amanda Oehlert, Ali Pourmand, Alexandre Gatineau, Kathy Panechou-Pulcherie, Patricia Blackwelder, CASSANDRA GASTON, *University of Miami*

Phosphorus (P) deposition from aerosols is important for bolstering primary productivity in nutrient-depleted ecosystems, leading to sequestration of atmospheric carbon dioxide. Transported Saharan dust is thought to relieve P limitation in Amazonian soil and the surface layer of the Tropical Atlantic Ocean (TAO) in boreal Spring, when Saharan dust transport is at an annual maximum. Alleviating these P limitations depends critically on the aerosol source and the P solubility, which determines how accessible P is for metabolic processes that stimulate primary production, particularly in the oceans. An important source of soluble P that is also transported to both the TAO and the Amazon Basin is biomass burning (BB) aerosol from Africa; however, this source is assumed to not be as important for relieving P limitations as African dust. We measured total and soluble P in long-range transported aerosols collected in Cayenne, French Guiana at a coastal site near the TAO and Amazon. Our measurements confirm that Saharan dust supplies P during boreal Spring, but the P solubility is only 5%. In boreal Fall when dust transport to South America is low, we measured unexpectedly high concentrations of total and soluble P, which we show are associated with transported BB from southern Africa. By extrapolating our results using a transport model, we show that African BB supplies up to half of P deposited to the Amazon. This is the first observational study to link P-rich BB from southern Africa to increased P deposition in the Amazon. Further, we show that African BB is a more important source of soluble P than dust to the TAO and may be more important for marine productivity in the TAO and oceans in the southern hemisphere, particularly in Summer and Fall.

7BC.6

What Matters for the Climate Impact of Biomass Burning Smoke. DANIEL MURPHY, *NOAA ESRL*

Biomass burning smoke is one of the largest and most diverse sources of aerosol in the atmosphere. I will provide an overview of how the radiative properties of smoke affect climate. If there is one message it is that simple radiative transfer calculations do not capture the climate impact of black or brown carbon. The concept of “adjusted radiative forcing” is crucial to understanding the climate impact of smoke. Even the sign can change: in some locations black carbon cools the Earth. Smoke is neither purely scattering nor black, it has multiple light-absorbing species, and is often injected above the surface. Each of these properties of smoke can have important implications for the radiative impacts. For example, altitude affects the radiative impact of an absorbing aerosol much more than it affects a purely scattering aerosol. That implies that the same smoke, containing both scattering and absorbing aerosol, can be net cooling if it is at one altitude and net warming at another.

7HA.1**Black Carbon Exposure during Physical Activity is Associated with Exhaled Markers of Oxidative Stress and Metabolomic Features Involving Oxidative Stress Mediating Pathways.**

ROBY GREENWALD, Matthew J. Hayat, Elizabeth Finlon, Donghai Liang, Jeremy A. Sarnat, Dean P. Jones, Parinya Panuwet, Lou Ann Brown, *Georgia State University*

The Study of Air Pollution and Physical Activity measured particulate matter exposure in adolescents and young adults participating in sports programs. We examined biomarkers of airway oxidative stress in exhaled breath, and in a subset of participants, we also conducted a Metabolome-Wide Association Study (MWAS) based on saliva samples collected pre- and post-exposure. We sampled at athletic fields in the Atlanta metropolitan area both near- and far from roadways, and we assessed particulate exposure in terms of PM_{2.5}, particle number concentration, and black carbon concentration (BC). These exposures were modest compared to many other Atlanta-area studies. We calculated the inhaled dose of pollutants using a validated method based on heart rate, breathing rate, and lung capacity. Exhaled biomarkers included expired nitric oxide (eNO) and malondialdehyde (MDA, a marker of lipid peroxidation) and glutathione (both oxidized and reduced) measured in samples of exhaled breath condensate. We observed significant positive associations between eNO and the inhaled dose of BC; however, this was not conclusive for other particulates or ozone. MDA was strongly associated with PM_{2.5} exposure in the previous 24 hours. Oxidized glutathione was negatively associated with the heat index during exposure but was not associated with any pollutants. MWAS results indicated associations between the body-weight normalized inhaled dose of BC and pathways related to leukotriene, arginine, and glutathione metabolism. These biological pathways have been associated with traffic-related air pollution in numerous studies. In addition, the previous 24 hour exposure to PM_{2.5} was also associated with leukotriene metabolism. These findings reflect the timing of sample collection immediately following a modest acute exposure. Exhaled biomarkers reflecting airway chemistry might be expected to respond within this time frame to acute exposures, but salivary biomarkers reflecting systemic processes may be more responsive to exposures hours or more in the past.

7HA.2**Air Pollutant Exposure and inhaled Dose during Urban Commute.** Keith Casserly, HAIDER KHWAJA, *University at Albany*

The prevalent environmental risk to health worldwide is air pollution. Increasing mortality and morbidity associated with polluted air has been epidemiologically demonstrated throughout the world. Particulate matter (PM) and black carbon (BC) found in polluted air has proven to be a powerful compromising agent of poor health by infiltrating the lungs and cardiovascular system, triggering diseases such as respiratory infections, stroke, lung cancer, heart disease and chronic obstructive pulmonary diseases. The aim of this study is to assess and map the exposure of commuters to air pollutants using different modes and to consider ventilation variability and travel duration for the estimation of inhaled dose. Particulate matter (PM₁, PM_{2.5}, PM₇, PM₁₀, and TSP) and BC were measured in the Capital District of Albany using four distinct modes of transportation viz., bicycle, walking, bus, and car. Data for pollutants revealed substantial transportation mode variations and temporal variation within and across study days. All transportation modes constitutively encountered the highest PM_{2.5}, PM₁₀, and BC concentrations in comparison to the other modes of transportation and the passenger car encountered the least. Although spatial variability was high within individual routes, average spatial variability between routes was less significant than diurnal variability for both PM_{2.5}, PM₁₀, and BC concentrations within the Capital region. Reduced exposure of pedestrian to air pollutants is compensated by their higher inhalation dose.

7HA.3

Sources and Health Risks of Ambient Polycyclic Aromatic Hydrocarbons in India. Fenglin Han, Hao Guo, Jianlin Hu, Sri Kota, Jie Zhang, Qi Ying, HONGLIANG ZHANG, *Louisiana State University*

Polycyclic aromatic hydrocarbons (PAHs) in the environment are of significant concern due to their high toxicity that may result in adverse health effects. PAHs measurements at the limited air quality monitoring stations alone are insufficient to gain a complete concept of ambient PAH levels. This study simulates the concentrations of PAHs in India and identifies the major emission sources. Annual anthropogenic emissions of CO, NO_x, SO₂, non-methane volatile organic compounds (NMVOC), PM_{2.5}, PM₁₀, EC and OC with a spatial resolution of 0.1° × 0.1° were downloaded from Emissions Database for Global Atmospheric Research (EDGAR) version 4.3.

Representative profiles for each EDGAR source category were taken from the SPECIATE 4.3 database. Biogenic emissions were generated using the Model for Emissions of Gases and Aerosols from Nature (MEGAN) v2.1. Open biomass burning emissions were generated from the Fire Inventory from NCAR (FINN). PAH emissions of 16 priority PAH species directly associated with health risks were generated from the global high-resolution PKU-FUEL-2007 inventory. The estimated emissions were then applied to simulate ambient concentrations of PAHs in India for January, April, July and October 2015 using the Community Multiscale Air Quality (CMAQ) model (v5.0.1). The spatial and temporal variations were analyzed and contributions of both local and regional major sources were quantified. Incremental lifetime cancer risk (ILCR) of exposure to NAPH and carcinogenic PAHs were also quantified to estimate the excess cancer cases in India. Source apportionment of ILCR was analyzed to represent contributions of different sectors. This study provides important information for the prevention and treatment of PAHs in India.

7HA.4

Quantifying Pharmaceutical Aerosol Dissolution at Relative Humidities >99.5%. ALLEN E. HADDRELL, Grazia Rovelli, David Lewis, Tanya Church, Jonathan P. Reid, *University of Bristol*

The efficacy of an inhaled pharmaceutical aerosol is dependent on the size and structure of the aerosol particles at the point of inhalation, its composition, and the microphysical processes that occur during inhalation. The degree to which/if particles grow when inhaled directly affects both where the dose is delivered and particle/droplet structure upon deposition. An understanding of this dynamic behaviour is critical to predicting regional and total dose, drug uptake, and pharmacokinetic rates. To be presented here is a comprehensive approach to probe all of these dynamic processes simultaneously for individual droplets produced from MDI, DPI and nebulizer starting formulations.

To study these effects, a new electrodynamic trap is to be reported. Novel features of the this trap include: (1) can capture and probe both liquid (originating from an MDI starting formulation or a nebulizer starting formulation) and solid particles (from a DPI starting formulation), (2) the conditions (relative humidity and temperature) that the levitated droplet experiences can rapidly be changed, (3) relative humidities greater than 99.5% are readily accessible. Taken together, these features directly mimic the conditions an inhaled aerosol experiences while simultaneously monitoring changes in particle size/structure.

Saturation is reached in the trap through creating a temperature gradient across the trapping region through independently controlling the temperature of each electrode with a Peltier cooler. The effect of changing the magnitude of the temperature gradient on water droplet evaporation is tailorable such that a relative humidity at saturation is readily reached.

This new trap is coupled with the a recently developed method to extract particle structure from light scattered from the droplet (termed a phase function). Together, these techniques allow for the detailed kinetic measurements of both droplet drying and dissolution to be reported.

7HA.5

Compositional Changes and Gas-Particle Partitioning of Unflavored E-Cigarette Carrier Liquids Propylene Glycol and Glycerol. SARAH SUDA PETTERS, Yael-Natalie Escobar, Grace Nipp, Yue Zhang, Tianqu Cui, Ilona Jaspers, Jonathan Thornburg, Jason Surratt, *University of North Carolina at Chapel Hill*

Since their introduction to the market in 2007, electronic cigarettes (e-cigarettes) have been widely adopted as a potentially safer alternative to tobacco cigarettes. Developing suitable techniques to study the long-term health effects of e-cigarette aerosol exposure is important because e-cigarettes are a relatively new and poorly characterized phenomenon with a growing market share. E-cigarettes generate aerosols by vaporizing a mixture of polyols, typically containing nicotine and flavor additives, in a heated cell, and then routing the saturated mixture to the mouthpiece, where it cools and forms a cloud of droplets. In this work we characterize the composition and gas-particle partitioning of e-cigarette aerosols. Unflavored solvents composed of propylene glycol (PG) and glycerol (GLY) were atomized in PG:GLY ratios of 0:100, 20:80, 35:65, 50:50, 65:35, and 100:0. Two different atomization methods were employed: pneumatic atomization at room temperature and heated atomization using a commercially-available e-cigarette device. Filter samples of the undiluted aerosol were collected and extracted in methanol. PG, GLY, and speciated oligomeric products were identified using reverse-phase liquid chromatography (RPLC) and hydrophilic interaction liquid chromatography (HILIC) coupled with electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (ESI-HR-QTOFMS). Gas-particle partitioning for different permutations of PG:GLY was quantified by RPLC/ESI-HR-QTOFMS and modeled using a binary evaporation model with UNIFAC activity coefficients. Results show that the nascent aerosol equilibrates quickly and partitions to first order according to its liquid PG:GLY ratio. Dimers and trimers of PG and GLY were identified in samples. These oligomeric degradation products generated from common carrier liquids, if specific to e-cigarettes, have the potential to serve as biomarkers in studies assessing the health impacts of e-cigarette aerosols.

7HA.6

Amorphous Pullulan Trehalose Microparticle Platform for Respiratory Delivery. NICHOLAS B. CARRIGY, Mani Ordoubadi, Yushan Liu, Omar Melhem, David Barona, Hui Wang, Leanne Milburn, Conor A. Ruzycski, Warren H. Finlay, Reinhard Vehring, *University of Alberta*

Spray drying consists of liquid atomization into droplets in a high flow of hot drying gas to evaporate the solvent and generate solid microparticles from the solutes. Relative to liquid dosage forms, solid dosage forms of spray dried powder tend to have improved thermal stability and lower storage space requirements, potentially allowing for widespread distribution to developing countries without cold chain infrastructure. Recently, it has been demonstrated that use of pullulan and trehalose as excipients outperformed use of leucine and trehalose for stabilizing *Campylobacter* bacteriophage in spray dried powder. Here, spray drying is used to generate inhalable pullulan trehalose powder that is characterized in terms of manufacturability, physical stability, device compatibility, and aerosol performance. Reasonable spray drying yield and powder flowability demonstrate the manufacturability. Short-term physical stability was evident as the powder maintained its amorphous phase during ambient temperature storage in a dry box and 40°C storage in pressurized metered-dose inhaler canisters containing commercial propellants HFA 134a and HFA 227, and subsequent actuation. The powder was theoretically predicted and experimentally supported to have a higher glass transition temperature near the surface, where biologics are expected to reside, than in the interior. Accurate predictions of particle diameter could be made using a newly developed particle formation model. The powder had suitable aerosol performance from a commercial dry powder inhaler as demonstrated by high dispersibility, optimal size for inhalation, and adequate total lung dose, exceeding many commercial inhalation devices. The non-reducing sugar-only and fully amorphous pullulan trehalose platform thus appears promising for respiratory delivery.

7IM.1

A Two-Stage Condenser to Improve the Detection of Sub-3 nm Particles Using Diethylene Glycol Condensation Particle Counter. Mo Xue, Michel Attoui, JINGKUN JIANG, *Tsinghua University, Beijing, China*

To improve the detection of sub-3 nm particles using diethylene glycol condensation particle counter (DEG-CPC), increasing their activation efficiency and counting as many particles as possible are both important. Comparing to the conventional one stage condenser, a two-stage condenser with different temperature helps to enlarge the domain with high supersaturation of diethylene glycol vapor, and subsequently increasing the activation efficiency of sub-3 nm particles. In comparison to the sheath-capillary condenser design of ultrafine CPC (UCPC), CPC with the unsheathed condenser design has higher particle concentration by eliminating the dilution effect of sheath flow. In this study, a diethylene glycol CPC with unsheathed two-stage condenser (TS-CPC) was developed. Temperatures of the saturator and two stages of the condenser are 51°C, 2°C, and 20°C, respectively. A warmer temperature of the second stage helps to prevent homogeneous nucleation of diethylene glycol vapor. Aerosol flowrate in the TS-CPC condenser is 1 lpm, significantly higher than that used in the DEG-UCPC condenser, i.e., increasing the number of particles to be counted. The new TS-CPC was theoretically and experimentally evaluated. Theoretical analysis confirms this design expands the domain with high vapor supersaturation and increases the number of particles to be counted. 50% detection efficiency diameter, Dp50, for negative and positive charged tungsten oxide particles were measured to be ~1.5 nm and ~1.8 nm. In addition, we show that Dp50 increased from ~1.5 nm to ~3 nm when the temperature of the first stage was increased from 2 °C to 20 °C. Scanning the temperature of the first-stage offers additional benefits. Sequentially stepping every 2 °C from 2 °C to 20 °C is given as an example and stabilized detection efficiency was observed within ~36 seconds for each step.

7IM.2

A New Mobility Particle Size Spectrometer Capable of Measuring the Size Tange from 1.1 to 55nm. GERHARD STEINER, Joonas Vanhanen, Joonas Enroth, Lothar Keck, Minna Väkevä, *Grimm Aerosol Technik Ainring*

In order to understand the basic mechanisms of new particle formation (NPF) as well as the formation rate and growth rate of the particles (e.g. Kulmala et al., 2013), it is crucial to measure aerosol number size distributions starting from the sub 2 nm size range. Current state of the art aerosol instrumentation is capable of detecting particles down to almost 1 nm (Vanhanen et al. 2011, Jiang et al. 2011), but commercial electrical mobility spectrometers are still lacking the necessary sensitivity in the sub 2 nm size range (Kangasluoma et al. 2017).

In this study, the Airmodus A10 Particle Size Magnifier (PSM, Vanhanen et al. 2011) is combined with the Grimm SMPS+C system in order to increase its sensitivity for the particles in the size range < 4 nm. The system consists of a soft x-ray neutralizer (Grimm 5524-X), a short Differential Mobility Analyzer (Grimm S-DMA), the diethylene glycol-based PSM (Airmodus A10) and a butanol-based CPC (Grimm 5416). The S-DMA was operated with an aerosol sample flow rate of 2.5 L/min and a sheath flow rate of 10 L/min, allowing size distribution measurements from 1.1-55 nm. The Grimm 5416 CPC was operated at a modified aerosol inlet flowrate of 1 L/min. The system was characterized using monodisperse particles produced with the Grimm WOX generator 7860 and electrospray generated molecular mobility standards (Ude & Fernández de la Mora, 2005).

The first results show that the new SMPS+PSM is capable of detecting small molecular ions < 2nm originating from the ionizing processes in the soft x-ray neutralizer and with its scan time of < 1min also of tracking very fast nucleation events. We will give details about the instrument's specifications and its performance for laboratory and ambient aerosol number size distribution measurements.

7IM.3

Modification of a Water-Based 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 light-weight, compact, commercial water-based CPC (> 5 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.

7IM.4

Brownian Dynamics Simulation to Investigate the Performance of Half Mini DMA to Classify Sub-2 nm Particles. HUANG ZHANG, Girish Sharma, Pratim Biswas, *Washington University in St Louis*

The knowledge of sub-2 nm particles is critical in understanding the early stages of particle nucleation and growth in nanomaterial synthesis and atmospheric aerosol systems. The half mini DMA has shown its ability to classify sub-2 nm particles by overcoming the diffusion limitation. Previous work numerically studied the particle transportation behavior in the classification region of short-bullet half mini DMA¹. However, the particle diffusion loss in the inlet and outlet part may be more severe, since the inlet and outlet tube are ~ 60 mm and ~ 120 mm, as compared to 4 mm and 20 mm of the classification region length for short-bullet and long-bullet type respectively. In this presentation, results of Brownian dynamic (using Monte Carlo approaches) simulations are presented to investigate the particle transport behavior in three parts of the half mini DMA: inlet section, working section, and outlet section. First, COMSOL 5.3 is used to simulate the velocity profile and electric field in the three sections. Following this, particle trajectories are tracked by Monte Carlo simulation. Based on these particle trajectories, the transfer function of the half mini DMA is evaluated for different aerosol, and sheath flow rates. This transfer function is also compared to our previous work, where aerosol convective-diffusion equations were solved. By combining the particle trajectories in the three sections, penetration efficiency for the half mini DMA is calculated. Finally, a complete description of particle transport in the half mini DMA is presented, and suggestions for improvement in the design are proposed.

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7IM.5

Charging Fractions of Soot Aggregates. TYLER J. JOHNSON, Robert T. Nishida, Xiao Zhang, Jonathan Symonds, Jason S. Olfert, Adam M Boies, *University of Cambridge*

Aerosols composed of soot aggregates are common due to the abundance of combustion sources. These particles are often characterized using electrostatic techniques, such as a Differential Mobility Analyzer (DMA), which require the charge fractions of particles to be known. However, previous studies in this area are limited, and all utilized a tandem DMA (TDMA) system. While a few studies have measured the ratios of bipolar charging fractions for aggregates, to the author's knowledge, Xiao et al. (2012) is the only study to measure absolute charging fractions of aggregates. To overcome challenges of the TDMA charging studies, Johnson et al. (2018) introduced a new method for characterizing charge conditioners with spherical particles using an Aerodynamic Aerosol Classifier (AAC), which exploited the truly monodispersed particle source produced by the AAC at a high transmission efficiency.

This work expands on these previous studies by demonstrating that operating an AAC upstream of a TDMA system can be used to eliminate multiple charging effects in the upstream DMA, while generating a source of non-spherical particles before charge conditioning that is monodisperse in aerodynamic diameter, mobility diameter, and mass, and therefore morphology. Up to 13 charging fractions from a bipolar charge conditioner at seven different mobility diameters (between 79 and 424 nm) of soot aggregates are measured. These results show a higher portion of aggregates become multiply-charged than spherical particles at the same mobility diameter. These results demonstrate the current theory of bipolar charging does not capture the effects of particle morphology.

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7IM.6

An Aerosol Gas Exchange System (AGES) for Engine Exhaust Conditioning. MARKUS BAINSCCHAB, Sampsa Martikainen, Panu Karjalainen, Jorma Keskinen, Alexander Bergmann, *Graz University of Technology*

The current European Particle Number (PN) emission standard regulates the emission of non-volatile particles larger than 23 nm in diameter. In order to assess this quantity correctly, a sampling system has to remove condensable semivolatile compounds and inhibit growth of sub-cut size particles. State-of-the-art technologies tackle this task by diluting the sampled exhaust with hot air and subsequently providing residence time to the sample for evaporation (evaporation tube), oxidation (catalytic stripper) or adsorption (thermal denuder) of volatile compounds.

We present an Aerosol Gas Exchange System (AGES), which can be used as an alternative to for engine exhaust conditioning for particle number measurements. The system's core element is a counter flow denuder, which has previously been shown to provide effective removal of gaseous species from an aerosol while exhibiting limited particle losses. Diffusional transport through a porous membrane allows the exchange of gaseous compounds in the aerosol with a freely selectable purge gas. By integrating this device into a system comprising heaters, temperature measurement, flow control and pressure regulation, we provide an aerosol conditioning system that is applicable for a variety of sources at changing pressure and temperature conditions.

We performed laboratory-based experiments to test the AGES' capabilities in removing a variety of gaseous species that are abundant in engine exhaust. We altered the sample temperature and the flow rate to evaluate the impact of these parameters on the exchange performance of the system and fractional particle penetration. Additionally, we provide a detailed mathematical model and multiphysical simulations, which enable the prediction of the exchange efficiencies of untested substances.

The presented results demonstrate the potential of the AGES for engine exhaust conditioning amongst many other possible applications like atmospheric studies and aerosol mass spectrometry.

7RA.1

Evaluating Aerosol Property Predictions from E3SM Using Recent ARM Field Campaign Measurements in Continental and Tropical Environments. JEROME FAST, Po-Lun Ma, John Shilling, ManishKumar Shrivastava, Jason Tomlinson, Jian Wang, Rahul Zaveri, Alla Zelenyuk, *Pacific Northwest National Laboratory*

We use the DOE's new climate model, the Energy Exascale Earth System Model (E3SM), to simulate the evolution of aerosol populations during two recent Atmospheric Radiation Measurement (ARM) field campaigns: HI-SCALE and GoAmazon. The Holistic Interactions of Shallow Clouds, Aerosols, and Land-Ecosystems (HI-SCALE) campaign was conducted in north-central Oklahoma during spring and late summer Intensive Observation Periods (IOPs) of 2016 near the ARM Southern Great Plains (SGP) site. The Green Ocean Amazon (GoAmazon) campaign was conducted in the vicinity of Manaus during 2014 and 2015, with IOPs during the wet and dry season of 2014. Both campaigns had long-term ground measurements to complement more detailed aerosol property and precursor instrumentation onboard the G-1 aircraft during the IOPs to characterize aerosol mass, composition of single particles and bulk particle populations, and size distribution aloft. We use these measurements to evaluate predicted aerosol properties and their multi-day and seasonal variations made by the four-mode version of the Model Aerosol Model (MAM4) that is part of E3SM. In addition to quantifying model performance, we identify likely reasons for biases and their potential effect on aerosol-radiation-cloud-precipitation interactions. We also focus on secondary organic aerosol formation (SOA) processes since they are often the largest fraction of aerosol mass in both campaigns. The performance metrics between the two campaigns will be compared to assess how well the SOA treatment in MAM4 represents both continental and tropical environments. The global model predictions will also be compared with more detailed aerosol populations simulated by the regional WRF-Chem model that includes a sectional aerosol treatment and a more complex representation of SOA.

7RA.2

Intermediate-scale Concentrations of Volatile and Semivolatile Organic Compounds in the Near-canopy Forest Atmosphere and Implications for Emission Heterogeneity. JIANHUI YE, Carla E. Batista, Igor O. Ribeiro, Patricia C. Guimarães, Adan Medeiros, Rafael Barbosa, Rafael L. Oliveira, Sérgio Duvoisin Junior, Kolby Jardine, Dasa Gu, Alex Guenther, Karena McKinney, Leila Martins, Rodrigo Souza, Scot T. Martin, *Harvard University*

The emissions, deposition, and chemistry of volatile organic compounds (VOCs) are thought to be influenced by underlying landscape heterogeneity at intermediate horizontal scales of several hundred meters. Quantitative observations and scientific understanding at these scales, however, remain lacking, in large part due to a historical absence of facile observational approaches. Herein, horizontal heterogeneity in the concentrations of VOCs (e.g., isoprene and monoterpenes) and their corresponding oxidation products (semivolatile organic compounds, or SVOCs) over the near-canopy atmosphere was examined by sampling from a copter unmanned aerial vehicle in central Amazonia during the wet and dry seasons of 2018. Distinct VOC and SVOC concentrations were observed over two forest sub-types separated from one another by several hundred meters. A gradient transport model together with a large eddy simulation model was employed to investigate the relationship between variable VOC emissions from underlying forest sub-types and the observed concentrations of VOCs and SVOCs. The data set obtained from this study, linking the diversity among VOC emissions and atmospheric particulate matter production at intermediate scales, provides a better understanding of the ecological and Earth system roles of VOCs.

7RA.3

Atmospheric Microplastics in Populated and Remote Regions of Colorado. MARWA EL-SAYED, Katherine Benedict, Amy P. Sullivan, Bret Schichtel, Jeffrey Collett, *Colorado State University*

The topic of microplastic pollution has been targeted by many studies due to its adverse effects on marine, wildlife, and human health. However, these studies were primarily conducted in the marine environment, with limited studies investigating their presences in the atmosphere in Europe and China. To the best of our knowledge, this is the first study that characterizes atmospheric microplastics in the United States. Filters for analysis of microplastics were collected once a week during the spring and summer in Colorado in the western United States at two sites: Fort Collins and Rocky Mountain National Park which represent suburban and remote areas, respectively. Active and passive sampling were conducted simultaneously to determine both the concentration and the deposition rate of these atmospheric particles (number of particles per unit area per day). Blanks were taken regularly and precautions were instituted to prevent operator contamination of collection media and samples. Visual imaging of microplastics was performed using a light microscope to monitor their count and size. Microplastics were analyzed using Fourier Transform-Infrared (FTIR) spectroscopy in conjunction with an Attenuated Total Reflectance (ATR) accessory and a scanning electron microscope (SEM) coupled with energy dispersive X-ray spectroscopy (EDS). These analysis techniques allow us to gain insight into the chemical structure of microplastics in the atmosphere as well as prospective weathering processes responsible for their degradation. Preliminary results provide evidence for the presence of microplastics in different forms including: fragment, film, fiber, and pellet with comparable deposition rates to those reported in previous studies. The source(s) of these particles is examined to identify local versus long-range transport influences.

7RA.4

Characteristics of Particle Size Distributions for Two Sites in New York State. JOSEPH P. MARTO, James Schwab, Fangqun Yu, Gan Luo, *University at Albany, SUNY*

Atmospheric particulate matter (PM) is known to influence air quality, as a pollutant itself and through direct and indirect roles it plays in the atmosphere for formation of cloud condensation nuclei and providing surface for atmospheric chemistry. Direct observation of particle size distributions (PSDs) for PM allows for insight into the processes controlling PM such as localized formation due to new particle formation (NPF) events, internal processing due to coagulation and condensation, and transport from local and regional pollutant sources. While these processes are consistently happening to PM within the troposphere, their individual strengths vary dramatically with different atmospheric regimes. To explore the relative strengths of controls over PSDs, two field campaigns were performed at sites in New York State, at rural Pinnacle State Park for April 2017-April 2018 and urban Queens College for May 2018-June 2019 using two instruments to capture continuous size distributions for particles between 5.6 nm-20 μm . Presented here are findings for the processes contributing to size, shape, amplitude and time evolution of the particle size distributions, and how they vary between sites and seasonally within each site.

7RA.5

Multi-Wavelength Optical Properties of Arctic Haze Aerosols in the Canadian High Arctic. PATRICK HAYES, Andy Vicente-Luis, Samantha Tremblay, Rachel Chang, Pierre Fogal, Felicia Kolonjari, Sangeeta Sharma, Richard Leaitch, Alireza Aslemund, Norman O'Neill, *Université de Montréal*

The Arctic presents particular challenges when assessing aerosol direct and indirect climate forcing because of relatively sparse measurements in this region. Therefore, in situ surface measurements that characterize aerosols in detail, including their size distribution and optical properties, are needed to improve understanding of the composition and radiative properties of the Arctic atmosphere, particularly in the remote High Arctic.

The Polar Environment Atmospheric Research Laboratory (PEARL, 80°N 86°W) is a unique site for studying aerosols due to its location far above the Arctic Circle. At PEARL, year-round measurements of aerosol size distribution as well as of aerosol light scattering and absorption at 405 and 870 nm have been performed since 2016. During winter and springtime when the atmosphere at PEARL is impacted by Arctic Haze, scattering and absorption coefficients are much higher compared to the summer, with hourly total extinction reaching levels of 30 and 10 Mm^{-1} for 405 and 870 nm, respectively. Several intrinsic optical properties have been calculated from the measurements including SSA values as well as the scattering and absorption Angstrom exponents. Furthermore, the apparent real and imaginary components of the refractive index were retrieved using Mie theory, and their ranges ($n = 1.65 - 1.81$ and $k = 0.002 - 0.012$ at 405 nm) indicate very weak intrinsic absorption compared to elemental carbon.

A number of systematic relationships are found between the different optical properties. For example, the SSA at 405 nm is generally higher than that determined at 870 nm, with values ranging between 0.95 – 1 and 0.80 – 0.95, respectively. The higher scattering efficiency at the shorter wavelength is attributed to the relatively fine particle size of Arctic Haze aerosol. Lastly, comparisons of the in situ measurements to remote sensing and model data will also be discussed.

7RA.6

Chemical Imaging of Atmospheric Particles Sampled over Agricultural Fields in Indiana. JAY TOMLIN, Kevin Jankowshi, Swarup China, Brian Stirm, Robert Kaeser, Paul Shepson, Alexander Laskin, *Purdue University*

The midwestern United States is a geographical region with large-scale agricultural fields. Crops in this region include corn, soybeans, and wheat among others, which all co-exist with a myriad of biological microorganisms (e.g. bacteria, yeasts, spores of actinomycetes and fungi, etc.). The harvesting of these crops aerosolizes biological particles and injects them into the atmosphere, contributing to the overall diversity of atmospheric particles in the area. A notable trait of airborne fungal spores is their ability to disintegrate into smaller particles upon hydration/dehydration cycles. This phenomenon is believed to have relevance to certain episodes of particle emissions reported over vegetated areas. Upon crop harvest, the aerosol mixing states and composition pertinent to these agricultural regions are disproportionately influenced by large amounts of fine plant fragments, soil dust, and biological spores released into the atmosphere. Resulted fine particles then travel long distances, depending on their size and the meteorological conditions. Recognizing the agricultural cycles in these regions, we can derive a predictive understanding of particle emissions in the local area. In this work, we collected ambient particles on board a research aircraft and sampled across agriculture fields and forests in the rural regions of Indiana. Collected samples were then analyzed using computer-controlled scanning electron microscope coupled with elemental microanalysis to describe particle-type population on statistically significant number of analyzed particles and Scanning Transmission X-ray Microscopy to provide quantitative metrics on particle internal heterogeneity. In addition, we used HYSPLIT dispersion modelling to provide insight into the complex transport and depositions of particles released from crop harvesting. Evaluating yet underrepresented sources for particle formation, such as biological particles and their fragments will contribute to improved inventories of atmospheric aerosols, essential to issues of climate, weather, and air quality.

7UA.1

High Resolution (1 km) Chemical Transport Modeling of Fine Particulate Matter in an Urban Area. PABLO GARCIA, Shayak Sengupta, Spyros Pandis, Peter Adams, *Carnegie Mellon University*

We undertake high resolution, 1 km chemical transport modeling of fine ($D_p < 2.5 \mu\text{m}$) particulate matter ($\text{PM}_{2.5}$) in Pittsburgh during winter of 2017 to quantify intra-urban and urban-rural gradients in $\text{PM}_{2.5}$ concentrations and composition. We use PMCAMx to simulate $\text{PM}_{2.5}$ treating aerosols across 10 particle size bins and organic aerosols with an additional 10 volatility bins. Traffic and restaurant activity significantly vary at the urban scale. Consequently, model inputs include new high resolution emissions inventories for traffic and cooking PM sources combining 2011 U.S. EPA National Emissions Inventory (NEI) estimates with a traffic model and restaurant locations, respectively. We evaluate model predictions with an aerosol mass spectrometer, an intra-urban network of Real-time, Affordable, Multi-Pollutant (RAMP) monitors and regulatory monitors from the EPA-CSN network. Average $\text{PM}_{2.5}$ predictions agree with RAMP observations with a mean fractional bias (MFB) of 13% and a mean fractional error (MFE) of 16% highlighting the ability of the models to resolve urban scale gradients. EPA-CSN measurements show an urban-rural gradient of $3.39 \mu\text{g m}^{-3}$ that agrees with the $3.56 \mu\text{g m}^{-3}$ predicted by PMCAMx, this highlights the ability of the model at reproducing regional concentration fields. We predict an organic aerosol (OA) fraction of the total PM of 54% compared with an observed fraction of 38%. Of this fraction the model predicts 98% to be primary, with an observed fraction of at least 81%. This suggest that OA emissions, including cooking, are over-estimated in the inventory.

7UA.2

PM_{2.5}, PM₁₀, and Ozone Forecasting in Southern California: Determining the Best Forecast Model as a Function of Predicted Meteorology and Emissions. SCOTT A. EPSTEIN, Nico Schulte, Mark Bassett, Elham Baranizadeh, Melissa Sheffer, *South Coast Air Quality Management District*

The South Coast Air Quality Management District is responsible for issuing a daily air quality forecast of $\text{PM}_{2.5}$, PM_{10} , ozone, carbon monoxide, and nitrogen dioxide for the counties of Los Angeles, Orange, Riverside, and San Bernardino—a region encompassing approximately 18 million residents and over 32,000 square miles. Daily forecasts are tailored to 45 individual areas for the following day and the day after that, with the addition of hourly air quality index predictions expected in summer of 2019. A combination of statistical and gridded chemical transport forecast models are used to make predictions for each pollutant on a 30 and 64 hour time-horizon. The models have prediction errors that are strongly related to location, emissions, and meteorology; differences in model structure and behavior lead to conditions where one model produces smaller errors than the others. Traditionally, an experienced forecaster identified the most reliable model for a particular day based on recent model errors.

To automate this task and reduce prediction errors, we developed an algorithm using feature selection methods to predict the root-mean-squared (RMS) prediction error of each model on the prediction day based on model performance on days with similar meteorology and emissions. A weighted distance-based regression is used to identify days in the previous year that are most similar to the prediction day. The algorithm then selects the model with the smallest RMS error at each of the 45 forecast areas for $\text{PM}_{2.5}$, PM_{10} , and ozone. Implementation of this algorithm leads to reduced RMS prediction error in all forecast regions throughout the entire year. The algorithm will be an important part of our plan to integrate additional forecast models into the forecasting system to further improve forecast accuracy.

7UA.3

Impacts of Spatial Distribution and Spatial Resolution of Emissions on Air Quality Model. YITING LI, Michael Kleeman, *University of California, Davis*

Air quality models are widely used to estimate human exposure to air pollution and to predict the health benefits of proposed emissions control programs. Air quality models predict pollutant spatial gradients that influence their overlap with human populations and therefore determine their public health impact. The accuracy of pollutant spatial fields is linked to: 1) the accuracy of the underlying emissions inventory, which often relies on spatial surrogates to determine where emissions occur within each county; and 2) the spatial resolution of the emissions inventory and air quality model, which affect the ability to capture concentration gradients around populated regions.

Here we study the impacts of emissions spatial distribution and spatial resolution on predicted pollutant concentration fields and the resulting air quality model performance. Several major surrogates are updated to improve the spatial distribution of emissions originally at 4km resolution. Surrogates including population, total housing, single-family housing, total employment, industrial employment, agricultural employment and service & commercial employment are created using high spatial resolution socio-economic data. The surrogate for construction equipment is updated using information from the California Water Resource Board NOI records and Caltrans' on-road construction database. The Longitudinal Employer-Household Dynamics database is used to update the surrogate for industrial equipment. These major surrogates are used to allocate area emissions at 1km resolution.

Simulations were conducted to evaluate if the updated spatial surrogates and downscaled emissions improved the accuracy of predicted particulate matter concentrations during past episodes. Model predictions for future episodes were also evaluated to determine if the two changes significantly affected population exposure to pollutants under various future energy scenarios. The goal of this research is to improve the accuracy of exposure calculations allowing for more detailed analysis of historical air pollution health impacts and more realistic analysis of changes to public health associated with future emissions reductions.

7UA.4

Simulation on IVOC Emissions and SOA Formation in Los Angeles during CalNex Study Using Updated Mobile Source Emission Profiles and SOA Parameterization. Quanyang Lu, Benjamin Murphy, Peter Adams, Yunliang Zhao, Momei Qin, Havala Pye, Christos Efstathiou, Chris Allen, ALLEN ROBINSON, *Carnegie Mellon University*

In this talk, we describe simulations using Community Multiscale Air Quality model version 5.3 (CMAQ v5.3) to investigate the contribution of intermediate volatile organic compounds (IVOCs) to secondary organic aerosol formation (SOA) in Southern California during the CalNex study. We first derive a simplified parameterization for SOA formation from IVOCs that accounts for both differences in volatility and molecular structure. We also implement new mobile emission profiles that quantitatively include IVOCs based on direct measurements. In the Los Angeles region, gasoline sources emit four times more non-methane organic gases (NMOG) than diesels, but diesel emit roughly three times more IVOCs on an absolute basis. All mobile sources (including on- and off-road gasoline, aircraft and on- and off-road diesel) are predicted to contribute 2.4 $\mu\text{g}/\text{m}^3$ of hydrocarbon IVOCs in Pasadena, CA, which corresponds to 38% of the concentrations measured during the CalNex campaign. Therefore, mobile sources emissions do not explain the total measured hydrocarbon IVOCs. To close the mass balance in Pasadena, IVOC would need to contribute 12% NMOG emissions from non-mobile sources. Mobile and non-mobile source IVOCs increase the model predicted SOA in Pasadena by a factor of 5.2. In a scenario with IVOC equal to 26.8% NMOG for non-mobile sources, modelled OA agrees well with the AMS-measured average OA diurnal pattern with noon peak SOA of 8.6 $\mu\text{g}/\text{m}^3$. In areas downwind of L.A., on average, 70% of predicted OA mass is SOA formed from oxidation of IVOC emissions. Evaluating the model predicted OA using 24-hr average OC concentrations from the Chemical Speciation Network (CSN, assuming OA-to-OC ratio = 1.8) shows that, with added IVOC emissions, the overall Fractional Bias (FB) is reduced from -0.59 to -0.10 and the Fractional Error (FE) is reduced from 0.67 to 0.42 for 7 sites in California.

7UA.5

Estimated Aerosol Radiative and Health Effects of the Residential Coal Ban in the Beijing-Tianjin-Hebei Region of China. KELSEY BILSBACK, Michael Cheeseman, Bonne Ford, Jack Kodros, Xiaoying Li, Emily Ramnarine, Ellison Carter, Jeffrey R. Pierce, *Colorado State University*

Particle-phase air pollution is a leading risk factor for premature death globally and impacts climate by scattering or absorbing radiation and changing cloud properties. In the Beijing-Tianjin-Hebei (BTH) region of China, where there are severe air quality problems, the government is implementing a ban on household use of coal for space heating, coupled with a subsidy for electric- or gas-powered heat pumps. We used the GEOS-Chem-TOMAS model, at $0.25^\circ \times 0.3125^\circ$ resolution to evaluate the potential impacts of this policy on air quality, mortality, and climate. We quantified the impacts of two different scenarios: (1) a complete heating transition in the Beijing province only and (2) a complete heating transition in all the BTH provinces. We estimate that 2,200 (interquartile range = 1,500-3,000) premature deaths will be avoided annually in the Beijing-transition case and 16,600 (11,100-23,200) in the BTH-transition case. However, these numbers represent a small fraction of the total annual premature deaths associated with air pollution across China (approximately one million), because the average $PM_{2.5}$ levels remain high even after residential coal combustion is removed as a source (and $PM_{2.5}$ levels are unaffected in other regions in China). We also estimated a positive direct radiative effect (DRE), with both an external and internal mixing assumption, and a positive cloud-albedo indirect effect (AIE) in the Beijing-transition case (maximum value in any gridbox for external DRE: $+0.18 \text{ W/m}^2$; internal DRE: $+0.15 \text{ W/m}^2$; AIE: $+0.07 \text{ W/m}^2$) and the BTH-transition case (max external DRE = $+1.16 \text{ W/m}^2$; internal DRE: $+1.00 \text{ W/m}^2$; AIE: $+0.25 \text{ W/m}^2$). However, the warming tendency from both the DRE and AIE were small and only affect winter heating months.

7UA.6

Bridging Model Estimates of Vehicular Emissions with Near-Roadway Ambient Measurements. AYLA MORETTI, David R. Cocker III, Matthew Barth, *University of California, Riverside*

Currently, vehicle emissions are measured using dynamometers and/or portable emissions measurement systems (PEMS); however, these systems operate at temperature and dilution ratios not representative of the ambient atmosphere. Estimates of near-roadway particulate matter (PM) concentrations using these emission factors within emission models, such as the EPA's Motor Vehicle Emission Simulator (MOVES), underpredicts measured near-roadway PM concentrations. A majority of differences between the near-road ambient studies and MOVES could be due to the changes in PM that occur immediately after the emissions rapidly dilute and cool in the ambient atmosphere. Evolution of engine technology, emissions control technology, and fuel composition further motivates the need to revisit effects of dilution and cooling on engine exhaust.

Organic aerosol (OA) formation from gasoline vehicle emissions were measured with a temperature controlled dilution sampler to account for additional OA formation during the dilution and cooling process, on the timescale of near-roadway emissions. The dilution sampler simulates the rapid dilution and cooling that occurs as the vehicle exhaust mixes with the ambient atmosphere following the original approach of Hildemann et al. (1989). The emission factor of a small gasoline engine was measured as a function of dilution and residence time to assess the sensitivity of the emission factors to near-roadway meteorology. A new module within MOVES was developed using ratios of measured (after dilution) emission factor to chassis and PEMS emission factors to identify the sensitivity of the near-roadway PM estimation from tailpipe to dilution processes. Characterization of the diluted aerosol include aerosol sizing (SMPS), aerosol shape and density (APM-SMPS), volatility (v -TDMA), and bulk chemical composition (HR-ToF-AMS).

8AE/IA.1**An Analysis of Fine Inorganic Aerosols Emitted by a Diesel Engine with Urea-Based Selective Catalytic Reduction.**

TERESA BARONE, Taekhee Lee, Jon Hummer, Sherri Friend, John Storey, Samuel Lewis, Aleksandar Bugarski, *National Institute for Occupational Safety and Health*

Exposure to diesel exhaust may adversely affect cardiovascular health and increase risk of lung cancer. Diesel exhaust exposures can be reduced through the application of emissions control strategies. One strategy for diesel equipment in the construction, agriculture, and mining industries involves high-temperature combustion and urea-based selective catalytic reduction (urea-SCR). Adequate performance of the urea-SCR system is necessary to prevent worker exposure to acutely toxic NO₂ in confined working spaces. Aerosol emissions that may hinder urea-SCR performance were investigated by size-separating and collecting 0.03-10 μm aerosols with an electrical low-pressure impactor. Aerosols were sampled isokinetically near the urea-SCR outlet and were analyzed by scanning electron microscopy and energy dispersive x-ray spectroscopy. The samples were collected from a medium-duty off-road engine, which was operated at mid-speed (1400 rpm) and high-load (530 ft-lbs) on an engine dynamometer. The system utilized commercially available diesel exhaust fluid (DEF) for urea-SCR operation that consisted of 32.5% urea in water. Aerosols collected after the urea-SCR system were predominately soot aggregates in the ultrafine size range ($\leq 0.1 \mu\text{m}$). However in the fine size range ($\leq 2.5 \mu\text{m}$), inorganic aerosols were abundant. They consisted of spherical particles of calcium, phosphorus and iron and irregularly shaped particles of sodium and iron. Fine inorganic aerosols may have originated from the use of DEF and engine lubricating oil. They are detrimental because they may deposit in the catalyst system and reduce catalyst performance. Their prevalence suggests that DEF impurities and lubricating oil additives should be limited to avoid urea-SCR catalyst fouling and consequently to prevent exposure to acutely toxic NO₂ in confined working spaces.

8AE/IA.2**Establishment of a PM Toxicity Evaluation Platform for Tailpipe Emissions under Real Driving Conditions.**

CHEN-HUA WANG, Yi-Ying Chen, Po-Kai Chang, Hsiao-Chi Chuang, Ta-Chih Hsiao, *National Taiwan University, Taiwan*

Several studies have shown that exposure to particulate matter correlates with cardiovascular and pulmonary diseases. The particles upon inhalation lead to local cellular reactions in the lung tissue, such as oxidative stress and direct cytotoxic effects. Traffic related combustion processes, like gasoline and diesel engine, are major contributors to these pollutions. The exhaust emissions from these engines are influenced by driving speed, acceleration and deceleration, ambient temperature, and engine operating temperature. Since dynamometer testing under laboratory conditions suffers from non-representativeness of actual driving conditions, lots of researchers use portable instruments to measure the pollutants under the real states. However, to the best of our knowledge, few studies provide the toxicological data of these. Hence, the purpose of this study is to establish a PM toxicity evaluation platform for tailpipe emissions under disparate real driving conditions.

The second version of On-Board Diagnostic system (OBDII system) and portable instruments were used to carried out on-board tests. The system was used to measure engine parameters over time. Combining the vehicle data with quantity of emissions measured by the instruments, the variety of concentrations of black carbon, particulate matter (PM), and gases were analyzed in real traffic situations. Simultaneously, the lab-made electrostatic precipitation air-liquid interface (ESP-ALI) exposure system was used to perform cell toxicity tests. Cytotoxicity tests were implemented by assessing the viability of human monocytic cell line (THP-1). Also, oxidative potential of the PM was assessed through the cell-free dithiothreitol (DDT) assay. The details of the PM toxicity evaluation platform, cell toxicity and oxidative potential of PM under real driving conditions will be given in this presentation.

8AE/IA.3

Online Aerosol Monitoring for In Vitro Toxicological Studies Using Single-Photoionization Mass Spectrometry. CARLA FREGE, Sandro Steiner, Sandra Ferreira, Shoaib Majeed, Francesco Lucci, Mahdi Asgari, Julia Hoeng, Stefan Frentzel, Arkadiusz Kuczaj, *Philip Morris International R&D*

Chemical and physical characterization of transported evolving aerosols in in vitro systems present a series of challenges, spanning from appropriate sampling ability of delivered aerosols through measurement capabilities of their properties to possibilities of performing online measurements of the compounds of interest in the flowing aerosol during exposure. In addition, when using mass spectrometry, high concentrations of compounds (in the range of parts per million) can saturate the detection system. Furthermore, the ionization method for detection of molecules of interest can produce fragmentation, making the analysis process more difficult. In this study, we used soft ionization mass spectrometry to measure the main compounds of e-cigarette aerosol online during in vitro exposure. A single-photoionization time-of-flight mass spectrometer (SPI-TOF-MS) (F. Mühlberger et al., 2002) was used to measure the chemical composition of the aerosol. The initial e-cigarette test liquid (e-liquid) was composed of propylene glycol and glycerol, nicotine, and water. Aerosol flow was driven by the standard operating procedure (55 ml puff volume in 3 seconds, 30-second frequency) using a programmable dual syringe pump (WHO TobLabNet SOP1, 2012), and measurements were performed by sampling undiluted and diluted test aerosol by mixing it with pure air, sampled in a transfer line through a capillary with a flow rate of 2–4 mL/min. The sample is ionized by a deuterium lamp, and ions are guided through a set of lenses, where they are detected according to their time of flight. The applied technique opens the possibility not only to quantify compounds of interest during exposure but also to perform detailed time resolution of delivered aerosol on a puff-by-puff basis. The system can be applied to monitor targeted compounds in a specific mass-to-charge range (40–200 m/z). Complementary measurements are ongoing to further investigate the application of SPI-TOF-MS for online monitoring of in vitro exposures.

8AE/IA.4

Estimations of Oxidative Potential Contributed by Metal Oxides in Welding Fume Particles. JUN WANG, Jacob Bartels, Macrio Bezerra, *University of Oklahoma Health Sciences Center*

Welding fume particles containing metal oxides contribute to oxidative potential (OP) and subsequently oxidative stress and other health outcomes. Welders are potential victims of significant fume exposure. The contributions from fume particles to OP are critical for understanding the health effects and risks of fume exposure. Anti-oxidant-based dithiothreitol (DTT) and ascorbic acid (AA) assays were widely used in estimating chemical-based OP of ambient particulates. However, the composition and concentration of welding fume particles differ vastly from ambient particulates. The concentrations of welding fume particles in workplaces are typically several magnitudes higher than ambient particulates, which may lead to a much faster reaction rate with the anti-oxidants. The composition of welding fume particles is predominantly metal oxides. In this study, a preliminary assessment of the applicability of DTT and AA assays to welding fume particles were conducted. Welding fume was generated in a fume chamber and collected with high volume flow pumps. The samples were extracted with buffer solutions and diluted to acceptable ranges for ultraviolet and visible spectrometer. The consumption of DTT and AA were measured as their reaction products 2-nitro-5-thiobenzoic acid and ascorbate at absorbances of 415 nm and 265 nm, respectively. Oxidation levels of welding fume were measured using a previously developed protocol based on metal cation concentration. General linear model was used to assess the correlation of DTT, AA, and metal cations. The results showed DTT assay performed poorly with welding fume particles and 78% of samples were unable to produce statistical significance. The AA consumption rate is between 0.68 and 1.27 nmol AA/min/ μg of fume particles, which are substantially higher than the values reported in ambient particulate studies. The regression R value for AA with metal cations concentration is 0.67. Overall, AA assay performed superiorly than DTT assay with fewer steps involved.

8AE/IA.5

Lung Dosimetry Assessments of Welding Fume and Gas Exposure using a Virtual Human Model with a Subject-Specific Respiratory System. JIANAN ZHAO, Yu Feng, Macrio Bezerra, Jun Wang, Ted Sperry, *Oklahoma State University*

Welders are constantly exposed to airborne fumes and gases. Exposures to metallic particles and toxic gases generated by welding can lead to respiratory diseases, neurological ailments, and ultimately cancer. Hazard identification and risk assessment are necessary for constructing a health-friendly welding environment. Accurate information on the transport and deposition of metal aerosols in the respiratory system and skin absorption are critically needed for precise health risk assessments. However, measurements from human and animal studies are restricted by the limitations of imaging resolutions and operational flexibilities. To overcome the drawbacks of conventional investigation methods, the experimentally validated computational fluid-particle dynamics (CFPD) models can be the alternatives, which are capable of providing local lung deposition distributions based on the natural laws of physics in a noninvasive manner. In this study, a multiscale CFPD model was developed and applied to a virtual fabrication shop integrated with a virtual human in order to evaluate the effects of ventilation conditions, particle size, and gas species on lung uptake and skin absorption, as well as ambient distribution and deposition. Numerical results indicate that the ventilation condition can significantly influence welding gas transport and deposition. Besides, the air-tissue absorption coefficient is the key factor in pulmonary gas absorption. For metallic particles with diameters 100, 190, and 830 nm, total particle deposition fractions were less than 18.0%, and most of them deposited in the oral cavity. Furthermore, particles tend to penetrate to the two upper lobes more than the rest three lobes. In summary, a validated *in silico* investigative framework has been built. Welding particle and gases transmission, transport, and deposition have been simulated and analyzed from the emission source to the human respiratory system. This work paves the way to build a personalized virtual human and indoor environment for noninvasive precise health risk assessments.

8AE/IA.6

Passive Exposure to Aerosols Emitted from Vaping Marijuana Liquid. LANCE WALLACE, Wayne Ott, Kai-Chung Cheng, Tongke Zhao, Lynn M. Hildemann, *US EPA (retired)*

A popular method of inhaling marijuana is by heating marijuana oil (vaping). We study real-life PM_{1} , $PM_{2.5}$ and PM_{10} concentrations as well as ultrafine particle numbers in two inhabited homes and determine decay rates, source emissions, and volatile fraction of the aerosol. Each test was conducted in a closed-off room in the two homes. A Scanning Mobility Particle Sizer (SMPS) with water-based CPC (Model 3788, TSI) provided ultrafine particle counts between 3 and 100 nm. One or two pairs of optical PM monitors were employed: SidePaks (TSI) and PA-II (purpleair). The purpleair monitor provides data on five size categories between 0.3-10 μm . Monitors providing direct measurement of $PM_{2.5}$ mass were also employed: the Piezobalance (Kanomax). The Piezobalance also has the property of losing volatiles from its crystal after some time, allowing an estimate of volatility of the aerosol. Aerosols were also collected on a filter and weighed. CO was measured by an electrochemical device (Langan Instruments) to provide estimates of the air exchange rate. A single puff of the heated marijuana oil was sufficient to elevate ultrafine numbers to $>100000\text{ cm}^{-3}$, and $PM_{2.5}$ concentrations to $>100\text{ }\mu g/m^3$, remaining elevated for several hours. Decay rates were calculated for the ultrafine particles and for five size fractions and displayed a monotonic decrease with increasing diameter for the ultrafines and a monotonic increase with increasing diameter for the range from 0.3-10 μm . The estimates of source strength (mg/puff) from the direct measurements of mass (Piezobalance and gravimetric) were in the range of 1 to several mg/puff, similar to secondhand smoke from cigarettes. Air exchange rates in one room varied from 0.1 to 0.2 h⁻¹. Initial estimates of the volatile constituents ranged up to 20%.

8AE/IA.7

Cognitive Impacts of Exposure to Indoor Sources. Heather Schwartz-Narbonne, BOWEN DU, Marlie Tandoc, Michael Mack, Jeffrey Siegel, *University of Toronto*

Exposures to indoor aerosols have been directly and indirectly linked to a variety of acute and chronic health outcomes. Despite these links, global indoor air quality has not improved appreciably in past decades, largely because of the lack of regulation, public education, and the temporal disconnect between exposures and health impacts. An alternative model for improving indoor air would focus on cognitive function impacts. The literature has several studies on cognitive impacts of indoor air pollutants, but most focus on CO₂. This investigation focused specifically on essential oil diffusers, small scale ultrasonic humidifiers that atomize a mixture of water and essential oils and are used to produce a pleasant scent and also generate >1 mg/h of submicron aerosol. Test subjects (N=42) completed a computer-based higher-level cognitive battery in well-ventilated test offices. Each test subject was randomly assigned to a cell on the experimental matrix consisting of presence/absence of lemon-scented essential oil in an essential oil diffuser and presence/absence of a HEPA filtration unit in an operating a portable air cleaner. Temperature, relative humidity, CO₂, formaldehyde, and ozone were all continuously monitored and were consistent between experimental conditions and not elevated over background. Concentrations of particles (0.3-10 μm) were elevated by approximately a factor of five over background for both conditions when there was essential oil in the diffuser, and slightly diminished in both cases when the portable air cleaner filtration unit was present. The presence of essential oil also greatly increased (by a factor of 3-10) the concentrations of d-limonene and β-pinene in the test office. Differences in subject responses to specific cognitive tasks were apparent at the different experimental test conditions suggesting that both particles and VOCs can impact high-level cognitive function.

8AP.1

Non-equilibrium Effects in SOA Formation and Evaporation Investigated with an Advanced Kinetic Multi-layer Model of Gas-particle Interactions (KM-GAP 2.0). THOMAS BERKEMEIER, Manabu Shiraiwa, Nga Lee Ng, Ulrich Pöschl, *Max Planck Institute for Chemistry*

In the formation of secondary organic aerosol (SOA), spatial inhomogeneity in composition can arise by early condensation of low volatile compounds (LVOCs) and later condensation of semi-volatile organic compounds (SVOCs). Composition-dependence of the viscosity of SOA mixtures shows that high prevalence of LVOCs can be correlated with high particle viscosity. Conversely, inhomogeneity in composition might cause spatial patterns of viscosity within a single particle, which can further reinforce the departure from equilibrium gas-particle partitioning. For example, evaporation of higher volatility compounds at the surface can lead to formation of a low volatility, high viscosity surface crust that shields SVOCs from evaporation. This process might be enhanced by “vulcanization” effects through oligomerization in the particle phase. Furthermore, adsorptive uptake may occur through a “burying” mechanism that is facilitated by slow particle-phase diffusion and leads to non-equilibrium composition of organic aerosol.

We use an advanced kinetic multi-layer model of gas-particle interactions in aerosols and clouds (KM-GAP 2.0) to investigate these effects and evaluate their potential impact on atmospheric SOA formation. The new model setup involves self-generation of model code and solves some limitations encountered in previous studies: a dynamic layer splitting and merging algorithm enables accurate description of high viscosity systems under preservation of moderate computational expense and numerical convergence. Examples of how the updated model can be used are presented and come from formation and evaporation of Secondary Organic Aerosol (SOA), as well as heterogeneous atmospheric oxidation chemistry.

8AP.2

Phase Behavior and Surface Tension of Sea Spray Aerosol Droplets using Microfluidics. SHIHAO LIU, Lucy Nandy, Cari Dutcher, *University of Minnesota*

Sea spray aerosol (SSA) is one of the largest contributors of atmospheric aerosol particles worldwide. As chemically complex aqueous systems that include mixtures of biological, organic, and salt constituents, it is a challenge to predict the phase of sea spray aerosol as they age in the atmosphere, which impacts species uptake, equilibrium partitioning and optical properties. In addition, various components in SSA are surface active, leading to an impact on surface tension and cloud condensation nuclei (CCN) activity. In this work, microfluidics is used to study droplet phase and surface tension of aqueous systems containing sea spray aerosol samples and chemical mimics. For some systems, 3-methylglutaric acid is added, to further study the impact of organics on the aerosol properties. For the phase behavior study, the aqueous droplets are generated in microfluidic channels and stored in passive traps until dehydration. Different phase states of collected sea surface microlayer (SSML) samples, including two LLPS and two crystallization, are observed. The main sea-salts in the samples are separated to study the contribution of each salt, the effect of solute concentration, and solute molar ratios on the observed phase and internal heterogeneities. For the surface tension study, a high-throughput multi-layer microfluidic tensiometer is used. Bubbles are generated and deformed in the microfluidic channel, where the deformation is controlled by the elongational effect from the viscous fluid (deforming force) and surface tension (restoring force). Image analysis is applied to capture the edge of the bubbles and extract flow field information for surface tension calculation. By investigating phase transitions and surface properties of aged aerosols, this study informs the properties and fate of SSA in the atmosphere.

8AP.3

Utilizing a Sub-Micron Silicon Nitride Waveguide as Single Particle Aerosol Detector. ANTON BUCHBERGER, Paul Maierhofer, Martin Sagmeister, Victor Sidorov, Jochen Kraft, Alexander Bergmann, *Graz University of Technology*

We present first results of a novel particle detector utilizing the interaction of particles with the evanescent field at the surface of a sub-micron waveguide. The transmission mechanism of light in a guiding structure is based on total internal reflection at the interface of a high to a low refractive index medium. The electromagnetic field of light guided through the high index medium does not abruptly vanish at this interface, but decays exponentially with a certain penetration depth. Hence, a portion of the total electromagnetic field is transmitted in this so-called evanescent region where it can interact with analytes such as particles. Interaction occurs in the form of scattering and absorption, thereby changing the total transmitted power through the waveguide. This influence to the total transmission is weak for guiding structures in the size range of standard single mode fibers (8-10 μm). By tuning the dimensions of waveguide structures to the range of the wavelength of the transmitted light, the ratio of the evanescent field to the total field can be drastically increased, which enhances the sensor effect strongly. The total transmission of light through such a structure is highly sensitive to any kind of perturbation in the evanescent region, like e.g. aerosol particles.

For the proof of principle, we use a silicon nitride waveguide with sub-micron dimensions for detecting surface impacted PSL spheres utilizing their influence to the total transmission through the device. The guiding structure consists of a silicon nitride strip as high index medium surrounded by air and silicon dioxide as low index medium. First deposition experiments with PSL spheres in the size range between 0.2 and 1 μm feature a relative decrease of the total transmission in the order of a few percent per deposited particle, revealing the potential of waveguides as highly sensitive particle detectors.

8AP.4

What Slows the Freezing of Pentane Nanodroplets? Kehinde Ogunronbi, Sherwin Singer, BARBARA WYSLOUZIL, *The Ohio State University*

Freezing of straight chain n-alkanes has been extensively investigated in part because they are a ubiquitous component of bioorganic molecules and fuels, and they exhibit unique behavior, such as surface freezing above the bulk freezing point. Their high heat of fusion and chemical stability also make them desirable in energy storage applications. A well-known oddity is that the melt temperatures of the low carbon number ($C_4 < C_n < C_{11}$) n-alkanes do not increase evenly with carbon number, an effect that reflects the ability of even alkanes to pack more efficiently than odd alkanes. The degree to which alkanes can be supercooled also varies with chain length. In bulk samples the degree of supercooling achieved by n-alkanes with $15 \leq n \leq 60$, is close to zero. In contrast, emulsified droplets of n-alkanes can be supercooled by up to 32°C. The near-zero supercooling for bulk samples was attributed to the formation of a crystalline monolayer at the sample-air surface at temperatures up to ~3°C above the melt temperature, that then leads to surface-induced heterogeneous nucleation once the melt temperature is reached.

In our work, we study the freezing of n-alkane nanodroplets in a rapidly cooling flow. For $6 \leq n \leq 10$ we can form these droplets and watch them freeze in the ~0.250 milliseconds available. Furthermore, freezing kinetics are consistent with surface freezing followed by crystallization within the interior of the droplet. We observe a strong even-odd alternation in the degree of supercooling reached before the rapid stage of crystallization started. In contrast, for $n=5$ we do not observe freezing on the timescale of the experiment, despite reaching temperatures that are more than 60K below the melt point. Molecular dynamics simulations of the n-alkane liquid-vapor interface, suggest that this behavior is consistent with a decreased ability to form the surface frozen layer.

8AP.5

Predictions of Viscosity of Organic Aerosols by Volatility Distributions: Applications to Field Observations. YING LI, Douglas Day, Harald Stark, Jose-Luis Jimenez, Manabu Shiraiwa, *University of California, Irvine*

Volatility and viscosity are important properties of organic aerosols (OA), affecting aerosol processes such as gas-particle partitioning, new particle formation and evolution of size distribution. Chemical composition of OA is complex and molecular specificity is often unavailable, which makes viscosity predictions of OA challenging. Laboratory experiments have found that viscosity of pure compounds is inversely correlated with vapor pressure. The molecular corridor-based analysis of hundreds of OA components shows that compounds with lower volatility have higher glass transition temperature (T_g), at which the phase transition between amorphous solid and semi-solid states occurs (Shiraiwa et al., 2017). Motivated by the evidence of close relations between volatility and viscosity, in this study we develop parameterizations to predict T_g as a function of pure compound saturation mass concentration for compounds including oxygenated organic compounds as well as nitrogen- and sulfur-containing organic compounds. The new parameterization is applied to field observations of volatility distributions to predict viscosity. The prediction shows that organic particles are mostly liquid in background conditions of the Amazonian tropical forest and semi-solid at low relative humidity conditions in the southeastern US, consistent with the results of ambient particle phase state measurements. Predictions for the other seven global observation sites show the frequent occurrence of non-liquid phase state in organic aerosols. The relation between volatility and viscosity established in this study is helpful to estimate viscosity from volatility distributions measured in field observations and laboratory experiments. It can also be applied in the molecular corridor or volatility basis set approaches to improve OA simulations in chemical transport models, by consideration of effects of particle viscosity in OA formation and evolution.

References:

Shiraiwa, et al. (2017), Global distribution of particle phase state in atmospheric secondary organic aerosols, *Nat. Commun.*, 8:15002.

8AP.6

Spray Aerosol Production from Raindrop Impaction on Seawater and Soil Surfaces. Kaili Zhou, Shurong Wang, Xin Yang, XIAOFEI WANG, *Fudan University*

Spray aerosol is a major source of atmospheric aerosols, which play crucial roles in radiative forcing, cloud formation and human health. In the atmosphere, spray aerosols are mainly produced from bubble bursting. Most of bubbles in natural water are generated via wave breaking which is induced by wind. However, it is known that bubbles are also formed by impaction of raindrop on water surface. Spray aerosol can be produced from bursting of these bubbles. According to our knowledge, no study has reported the production flux of spray aerosol from impaction of raindrop on water surface. In addition, several recent studies have shown that raindrop impaction on soil can also produce spray aerosols. Thus, it is crucial to access the contribution of spray aerosol from raindrop impact on seawater or soil. In this study, we simulated raindrop impaction on seawater and soil surface in the laboratory. The production rate, as well as physical and chemical properties, of spray aerosols were measured and characterized in details. Their environmental impact was discussed.

8AP.7

Mass Absorption Cross Section and its Enhancement Factor for Internally Mixed Black Carbon Aggregates with varying Fractal Dimension. PAYTON BEELER, William Heinson, Rajan K. Chakrabarty, *Washington University in St. Louis*

Mass absorption cross section (MAC) of black carbon (BC) aggregates is an important parameter in many climate models. An underestimation of MAC of BC aggregates can lead to errors in the estimation of radiative forcing due to BC in the atmosphere. BC aggregates are produced by incomplete combustion of biomass and fossil fuels. Aggregates of BC monomers are formed through diffusion-limited cluster aggregation (DLCA) of BC monomers. Organic compounds can then coat the surface of the BC aggregates, which alter the aggregate's fractal morphology via capillary and surface tension forces. This leads to an increase in the fractal dimension of emitted BC aggregates as the amount of coating increases. This study generates aggregates using three aggregation mechanisms; DLCA ($D_f = 1.8$), percolation ($D_f = 2.5$), and face-centered cubic stacking ($D_f = 3$). The aggregates are then coated with refractory (absorbing) and non-refractory (non-absorbing) organics, and their optical properties are calculated using the Amsterdam discrete dipole approximation (ADDA). The MAC values of the coated aggregates are next calculated and compared against uncoated aggregates for determination of MAC enhancement factors across a large size range.

8BC.1

Long-Range Transport Mechanisms in East and Southeast Asia and Impacts on Size-Resolved Aerosol Composition: Contrasting High and Low Aerosol Loading Events. RACHEL BRAUN, Mojtaba Aghdam, Paola Bañaga, Grace Betito, Ma. Obiminda Cambaliza, Melliza Cruz, Genevieve Lorenzo, Alex MacDonald, James Simpas, Connor Stahl, Armin Sorooshian, *University of Arizona*

This work analyzes mechanisms of long-range transport of aerosol and aerosol chemical characteristics in and around East and Southeast Asia. Ground-based size-resolved aerosol measurements collected at the Manila Observatory in Metro Manila, Philippines from July - October 2018 were used to identify and contrast high and low aerosol loading events. Multiple data sources, including models, remote-sensing, and in situ measurements, are used to analyze the impacts of long-range aerosol transport on Metro Manila and the conditions at the local and synoptic scales facilitating this transport. Evidence of long-range transport of biomass burning aerosol from the Maritime Continent was identified through model results and the presence of biomass burning tracers (e.g. K, Rb) in the ground-based measurements. The impacts of emissions transported from continental East Asia are also identified; for one of the events analyzed, this transport was facilitated by the passage of a nearby typhoon. Changes in the aerosol size distributions, water-soluble chemical composition, and water-soluble organic aerosol were examined for the different cases. The events impacted by biomass burning transport had the overall highest concentration of water-soluble organic acids, while the events impacted by long-range transport from continental East Asia, showed high percent contributions from shorter chain dicarboxylic acids (i.e. oxalate). The low aerosol loading event was subject to a larger precipitation accumulation than the high aerosol events, indicative of the potential impact of wet scavenging as an aerosol sink in the study region. This low aerosol event was characterized by a larger relative contribution from supermicrometer aerosols and had a higher percent contribution from longer-chain dicarboxylic acids (i.e. maleate) to the water-soluble organic aerosol fraction. Results of this work have implications for better understanding the transport and chemical characteristics of aerosol in a highly-populated region that has thus far been difficult to measure through remote-sensing methods.

8BC.2

Where's the Mass: Why Might Field and Laboratory Studies on Aging of Biomass Burning Aerosols Disagree on Mass Enhancements? ANNA HODSHIRE, Ali Akherati, Matthew Alvarado, Benjamin Brown-Steiner, Shantanu Jathar, Jose-Luis Jimenez, Sonia Kreidenweis, Chantelle Lonsdale, Timothy Onasch, Amber Ortega, Jeffrey R. Pierce, *Colorado State University*

Biomass burning is a major source of atmospheric particulate matter (PM) with implications for health, climate, and air quality. As biomass burning plumes are transported downwind, the particles and vapors undergo chemical and physical aging. These aging processes can either increase or decrease total PM mass, but aging always causes changes in the PM composition (e.g. oxygen-to-carbon ratio). Field measurements of the evolution of mass with age range from decreases to increases, with most showing little to no change. Conversely, laboratory studies tend to show significant mass increases on average. Currently, there is no consensus on why field measurements tend to show little mass change, or why field and laboratory experiments give such different results for total particle mass but show similar rates of change in composition. We summarize available observations of aging smoke mass concentrations and composition markers and discuss four broad hypotheses to explain variability within and between field and laboratory campaigns: (1) variability in emissions and chemistry, (2) differences in dilution/entrainment, (3) losses in chambers and lines, and (4) differences in conditions selected as "time zero", the baseline from which changes are estimated. Hypothesis (1) is well known and has been the subject of intensive research. Hypothesis (2) can potentially lead to greater aerosol evaporation in the field than the laboratory. Hypothesis (3) suggests there are losses of precursor vapors potentially unaccounted for, which would lead to even greater mass enhancements for the laboratory system. Hypothesis (4) indicates that if a great deal of chemistry occurs rapidly within the plume (<10 minutes), field studies that can only measure >10 minutes after emission would miss this initial mass enhancement. We show examples of the anticipated impacts of hypotheses (2)-(4) with the aim to spur community interest and further research in these areas.

8BC.3

Simulating the Near-Source Forest Fire Plume Chemistry and Secondary Particle Formation Using SAM-ASP. Chantelle Lonsdale, MATTHEW ALVARADO, Anna Hodshire, Emily Ramnarine, Jeffrey R. Pierce, *AER*

Biomass burning is a major source of trace gases and aerosols that impact health, air quality and the climate. Three-dimensional Eulerian chemical transport models use estimates of the primary emissions from fires and can unphysically mix them across large-scale grid boxes, leading to incorrect estimates of the impact of biomass burning on health, air quality and the climate. Plume-scale process models allow for the examination of the chemical and physical transformations of trace gases and aerosols within biomass burning smoke plumes and to develop parameterizations of this aging process for coarser grid-scale models. Here we describe the coupled SAM-ASP plume-scale process model, which consists of coupling the Aerosol Simulation Program (ASP) with the large-eddy simulation model, System for Atmospheric Modelling (SAM). SAM-ASP is an advancement on ASP in that the plume turbulent mixing is calculated by SAM and allows the study of how the chemistry within the smoke plume changes vertically and horizontally. SAM-ASP calculates the oxidant concentrations for SOA chemistry using a fully interactive photochemical model rather than being specified at fixed concentrations. We show that the SAM-ASP model is able to correctly simulate the dilution of CO in a California chaparral smoke plume, as well as the chemical loss of NO_x, HONO, and NH₃ within the plume and the formation of PAN and O₃.

8BC.4

Rapid Transformations of Biomass Burning Particulate Emissions in the Near Field. ARTHUR J. SEDLACEK, Timothy Onasch, Kouji Adachi, W. Patrick Arnott, Peter Buseck, Qi Zhang, John Shilling, Mikhail Pekour, Sonya Collier, Shan Zhou, Andrew Freedman, Lawrence Kleinman, *Brookhaven National Lab*

Aerosols from biomass burning are recognized to perturb Earth's climate through the direct effect, the semi-direct effect, and indirect effects. Whether wildfires are determined to heat or cool the atmosphere depends on the abundance and refractive index of emitted primary particles and secondary aerosol species. Currently inputs for model calculations are often based upon measurements of fresh (nascent) aerosols. However, a growing body of experimental evidence is beginning to indicate that aerosols generated in biomass burning (BB) events undergo rapid changes in their chemical, microphysical, and optical properties. Such rapid change suggests caution in the use of near-field aerosol properties in far field radiative forcing calculations.

During the summer and fall of 2013, the Department of Energy's Atmospheric Radiation Measurement (ARM) program sponsored a coordinated field campaign that combined aircraft-based measurements with mountain top observations to investigate the near-field (< 5 hrs) as well as regional evolution of biomass-burning (BB) aerosol particles. This field campaign, known as BBOP (Biomass Burning Observation Project), represents the first time that the near-field evolution of BB aerosol particles has been exclusively targeted with research aircraft. For the wildfire flights (17 fires sampled, ~175 plumes), a Lagrangian sampling protocol was employed in which flight transects orthogonal to the plume direction were conducted at selected distances downwind of the source. The plume age was calculated using prevailing wind speed/direction and the assumption of a constant emission source during the sampling period.

We will present recent findings on the formation and evolution of tar balls, near field changes in aerosol chemical, microphysical, and optical properties, and on measurements from the Mt. Bachelor Observatory (MBO, ~ 2700k) in Central Oregon which provide complementary information on regional characteristics of wildfire plumes to the BBOP flight results.

8BC.5

Analysis of Unidentified Organic Species in Fresh and Aged Biomass-Burning Emissions Generated under Controlled Conditions. VERA SAMBUROVA, Deep Sengupta, Chiranjivi Bhattarai, Adam Watts, Hans Moosmuller, Andrey Khlystov, *Desert Research Institute*

Large quantities of organic compounds are emitted into the atmosphere every day from different sources. Emissions from wildland fires and biomass fuel use contribute significantly to regional air pollution events, global-scale radiative forcing, and climate change. Global inventories of black carbon (BC) and organic carbon (OC) particulate mass emitted from combustion show that almost 90% of total carbonaceous aerosol mass is emitted from biomass combustion and the major fraction of these emissions is generated during smoldering combustion.

While hundreds of biomass-burning compounds have been identified at the molecular level, the chemical, physical, and toxic nature of the bulk of these biomass burning OC emissions remains poorly understood. To understand the impact of these atmospheric organics on the environment and human health, it is essential to know their chemical nature. In the present study, gas- and particle-phase biomass-burning emissions from different types of biomass fuels, mainly peats, were quantitatively and qualitatively analyzed for their chemical composition. The fuels were burned under controlled conditions (e.g., relative humidity, dilution of emissions, fuel-moisture content) at a biomass-burning facility (Reno, NV, USA). Fresh biomass-burning emissions were aged in an oxidation flow reactor (Aerodyne Research Inc.), mimicking several days of atmospheric aging. Samples were extracted from TIGF filters (particle-phase species) and XAD resin cartridges (gas-phase species) with dichloromethane followed by acetone and the resulting extracts were quantitatively analyzed for more than 200 organic compounds using gas chromatography mass spectrometry (GC/MS). Subsequently, the aliquots of these extracts were analyzed using the full-scan GC/MS technique to characterize unidentified organic species in fresh and OFR-aged biomass-burning emissions.

8BC.6

Measured and Modeled SOA Formation from Biomass-Burning-Derived Precursors. KELLEY BARSANTI, Isaac Afreh, Jia Jiang, Lindsay Hatch, William P. L. Carter, Weihang Peng, David R. Cocker III, *University of California, Riverside*

Fires can emit high levels of trace gases, including nitrogen oxides (NO_x); semi-volatile/intermediate-volatility/volatile organic compounds (S/I/VOCs); and primary particulate matter (PM). Quantities and properties of emitted gaseous and particulate compounds are highly variable and largely dependent on burn conditions, as well as fuel type (composition and structure). During plume dilution, primary PM can evaporate, decreasing the amount of primary organic aerosol (POA) but adding reactive gases (e.g., S/I/VOCs). During plume evolution, S/I/VOCs react to form secondary organic aerosol (SOA). Thus, predictions of the net amount of OA in evolving fire plumes depend on both the chemistry and dynamics of the partitioning species and their precursors. In this work, we analyzed gaseous organic compounds emitted from laboratory fires during the 2016 FIREX campaign at the Missoula Fire Lab, in which diverse fuel types were burned. We modeled gas-phase chemistry of a subset of the measured compounds using the SAPRC gas-phase chemical mechanism and GECKO-A (Generator of Explicit Chemistry and Kinetics in the Atmosphere); we also performed box-model simulations of SOA formation based on both SAPRC and GECKO-A mechanisms. We used the SOA model predictions and published chamber data to identify a list of likely important but understudied compounds for SOA formation. Based on that list, we then selected a series of compounds for which we ran smog chamber experiments. We will present the modeling study results on SOA formation from substituted furans and fuel-dependent monoterpenes as a function of fuel type, as well as under different dilution conditions. We will also present measurement-model comparisons using the newly acquired chamber data.

8BC.7**Large Contribution of Oxygenated Aromatic Compounds in Biomass Burning Emissions to Secondary Organic Aerosol Formation.**

ALI AKHERATI, Charles He, Matthew Coggon, Abigail Koss, Carsten Warneke, Joost de Gouw, Christopher Cappa, Jeffrey R. Pierce, Michael Kleeman, Shantanu Jathar, *Colorado State University*

Biomass burning is the largest combustion source of organic compounds to the atmosphere. However, there are large uncertainties in how the gas-phase organic compounds chemically react in the light and dark atmosphere to form secondary organic aerosol (SOA). In this work, we used a state-of-the-science model to simulate the chemistry, thermodynamic properties, and microphysics of SOA arising from photochemical aging of biomass burning emissions. The chemistry and thermodynamic properties were modeled using the Statistical Oxidation Model (SOM) and the microphysics was modeled using the Two-Moment Aerosol Sectional (TOMAS) model. The initial concentrations of the SOA precursors were informed by the detailed speciation performed using a H_3O^+ -chemical ionization mass spectrometer. We developed new sets of parameterizations to represent the SOA formation from oxygenated aromatic (e.g., phenol, guaiacol) and heterocyclic (e.g., furan and substituted furans) compounds since they contribute substantially to high molecular weight emissions from biomass burning. SOM-TOMAS was applied to 9 chamber experiments performed on four different fuels under moderate to high NO_x conditions. Traditional SOA precursors such as single-ring aromatics, isoprene, and terpenes accounted for less than 10% of the measured SOA. In contrast, oxygenated aromatic compounds, with major contributions from phenols and substituted phenols, guaiacol, and cresol, were responsible for approximately three-quarters of the observed SOA. Heterocyclic species were not found to be important SOA precursors. Oxygenated aromatic compounds are short-lived species and are likely to play an important role in the near-field evolution of organic aerosol (OA). Ongoing work is focused on using the SOM-TOMAS model (i) to simulate the production of particulate organic nitrates (PONs) in chamber experiments performed with the NO_3 radical and (ii) to investigate where laboratory-based parameterizations can help explain the field-observed OA evolution in wildfire plumes.

8CM.1**A Novel In-stack Pre-cutter for Separating Droplets in Gas Streams Saturated with Water Vapor.**

Chih-Hsiang Chien, Joshua Udvardy, CHANG-YU WU, Zachery Emerson, Derek Sain, Leland Carlson, Vipin Varma, Cathe Kalisz, *University of Florida*

Current EPA guidance states that facilities required to measure filterable $\text{PM}_{2.5}$ in saturated or droplet-laden stacks should use EPA Method 5/5B and use the total filterable PM as a surrogate for filterable $\text{PM}_{2.5}$. However, these two methods have no size classifier and therefore a gravimetric assessment of the downstream filter yields a higher-than-true emission rate of $\text{PM}_{2.5}$. The limitations of the available test methods warrant the development of a new method. A novel in-stack pre-cutter comprised of an exchangeable nozzle, an impactor and an absorption pad, has been designed to isokinetically separate droplets $> 10 \mu\text{m}$. Computational fluid dynamics was applied to evaluate and optimize the prototype. An SST K-Omega turbulence model was adopted to solve for gas transport, while the aerosol was simulated using a discrete-phase model. Our study reveals that there are three factors to be considered. First, to isokinetically extract, the exchangeable nozzle is designed as a diffuser to reduce particle inertia and achieve a cut size of $10 \mu\text{m}$ in the downstream impactor. Our study shows that flow separation could occur in the diffuser and lead to ineffective velocity reduction, causing higher particle inertia than expected and thus a smaller cut size. An optimal combination of the nozzle's half-angle at 7 degrees and extended throat length of 3 cm was identified to reform the boundary layer and slow down the free stream, leading to a desired cut size. Second, while the flow direction in a conventional impactor for ambient sampling is along that of gravity, the flow direction in the stack is against gravity. A previous study reported a smaller cut size due to gravity while this present study shows that the opposing flow direction can lead to a slightly larger cut size. Third, the pre-cutter dimension was enlarged to prevent secondary impaction of particles.

8CM.2

Numerical Simulations of Inhomogeneous Current Density Effects on ESP Performance for Fly Ash and Mercury Sorbent Mixtures. ERIC MONSU LEE, Herek Clack, *Illinois Institute of Technology*

Injection of powdered activated carbon (PAC) upstream of electrostatic precipitators (ESPs) has been the most commonly used strategy for post-combustion mercury emissions control at coal-fired power plants. However, as PAC injection rate increases upstream of ESPs, the darkening filters with particulate matter (PM) samples collected downstream of ESPs indicates an unidentified performance anomaly. It has been hypothesized that injection of PAC can introduce unexpected heterogeneity to the PM collection process in ESPs as PAC differs greatly from fly ash in both physical and electrical properties and can potentially pose challenges to ESPs that were originally designed and operated for coal fly ash removal. A previous experimental study centering on the differential collection of PAC-fly ash admixtures shows increasing trends of unaccounted-for particles based on mass balances as PAC concentration increases in the PAC-fly ash admixtures. Furthermore, measurement of powder resistivity of the ESP-collected powder samples infers that the unaccountable particles becomes more PAC-concentrated as PAC concentration increases. The objective of the present study is to develop a numerical model using COMSOL Multiphysics™ and explore additional variables leading to the increasing mass of unaccountable particles as PAC concentration increases. A Euler-Lagrange numerical scheme enables the modeling of the cylindrical ESP used during the experimental study and allows for solving the interrelated physics, including Maxwell's electric field coupled with charge conservation, electro-hydrodynamics (EHD) induced flow field, and particle tracing affected by transient electric force, aerodynamic drag and gravitational forces. The model shows that PAC is more susceptible to the vortex flows induced by the inhomogeneous current density on the collection electrode. In addition, when considering mutual couplings between the EHD flow and the dispersed phase, PAC can induce higher rates of momentum transfer and lead to intensified vortex flows. The findings provide new evidence for explaining the increasing mass of PAC-concentrated unaccountable particles and thus the darkening PM filters as PAC concentration increases.

8CM.3

An Experimental Study on Airflow Patterns of Pleated Filters by Using the PIV Method. QINGFENG CAO, Seungkoo Kang, David Y. H. Pui, *University of Minnesota*

Pleated filters are widely used for industrial and residential applications. Their filtration efficiency is highly related to the airflow fields. An experimental method has been developed for measuring the flow patterns passing through pleated filters by using the Particle Image Velocimetry (PIV) method, which is an optical approach for instantaneous flow visualizations and velocity measurements. In the current experimental study, flow patterns and pressure drop across pleated filters with various pleat configurations of different flow regimes have been measured under our laboratory setup. Velocity and vorticity contours at both the upstream and downstream regions of the flow field were obtained. It was found that the pleat geometry impacts the downstream flow pattern more significantly than the upstream flow pattern. The obtained downstream flow distributions indicate lower permeability at the pleat tip region than the rest of the filter media, so that air tends to pass through the sides of the filter pleats instead of the pleat tip region. By increasing the pleat number, we discovered that when pleat geometry stays unchanged, similarity exists among downstream flow patterns of the pleated filters with different pleat numbers.

8CM.4**Respiratory Deposition of Ultrafine Welding Fume Particles.**

WEI-CHUNG SU, Yi Chen, Marcio Bezerra, Jun Wang, *University of Texas Health Science Center at Houston*

In this study, a mobile aerosol lung deposition apparatus (MALDA) was developed and applied to study the respiratory deposition of ultrafine welding fume particles for performance evaluation. A series of respiratory deposition experiments were carried out using the MALDA to investigate the deposition of ultrafine welding fume particles in different generations of human airways. The results showed that the fractional deposition of ultrafine welding fume particle in the human tracheobronchial airways down to the 9th airway generation could be readily, efficiently, and systematically measured by the MALDA. This result suggests that the newly developed MALDA has the potential to be used in real-world occupational settings to estimate respiratory deposition of ultrafine welding fume particles as well as for other workplace ultrafine particles.

8CM.5**Resonances in Laser Desorption/Ionization of Particle-Bound Metals Feature Remote Sensing of Ship Emissions.**

Johannes Passig, Julian Schade, Thomas Kröger-Badge, Robert Irsig, Hendryk Czech, Martin Sklorz, Lei Li, Xue Li, Zhen Zhou, Benjamin Stengel, Bert Buchholz, Thorsten Streibel, RALF ZIMMERMANN, *Helmholtz Zentrum München and University of Rostock*

Ship emissions are important contributors to global air pollution with strong climate and health effects. Large amounts of particle-bound organics, sulfur and metals are emitted, especially under operation with low-grade bunker fuels. The particles metal composition is source-specific for ships running on these fuels and can be evaluated via single-particle mass spectrometry (SPMS). However, ambiguity in source apportionment increases with long-range transport because of interferences and only weak signals from some of the marker metals.

We present a so-far unrecognized enhancement effect in laser desorption/ionization (LDI). It leads to substantially increased ion yields for particle-bound metals in single-particle mass spectrometry (SPMS). As in conventional SPMS, the technique allows on-line characterization and classification of individual airborne particles.

The increased sensitivity for metals considerably improves the detection and evaluation of ship emissions in ambient air. We demonstrate detection of residual metals in ship emissions, even many hours after switching the engine from bunker fuel to diesel operation. Based on the ionization enhancement, we detected ship plumes from >100 km distance and attributed them to individual ship passages using freely available data from air trajectories and automatic identification system of the ships. In conjunction with the evaluation of sulfur emissions, violations against sulfur limits in emission control areas are now detectable from a large distance.

8CM.6

A CFD Study of a Vegetative Barrier as a Near-Road Pollutant Mitigation Strategy: An Evaluation of CFD Modelling Techniques with Field Measurements. KHALED HASHAD, Xinwei Liu, Bo Yang, K. Max Zhang, Pradeep S. Prathibha, Jay R. Turner, Daniel Fleischer, *Cornell University*

Traffic related pollution is shown to have an adverse effect on human health. Vegetative barriers have shown the potential to act as a mitigation tool for traffic pollution. A vegetative barrier comprised from a combination of (100+) shrubs and trees was implemented in front of Saint Margret Mary (SMM) School in Louisville, KY. LiDAR and on site measurements provided Leaf Area Density (LAD) for the different vegetative species used, in addition to, detailed geometric information for each tree. Both those parameters were used to develop our Computational Fluid Dynamics (CFD) model. A hybrid approach was used in the CFD model where big and dense vegetation was modelled as standalone zones, while smaller and spatially close vegetation was clustered together. Our model accounted for both the aerodynamic and deposition effects that vegetation has on the flow and particles. This simulation is unique since it provides a site specific analysis for pollutant concentration. In addition to the buffer, nearby buildings, vegetation, and traffic were considered. On field measurements of wind speed and pollutant concentration (Ultra-fine particles) were obtained. Our CFD results showed good agreement with field measurement results. This validates our model and provides a CFD tool for future analysis that can be used to test the effectiveness of vegetative barrier designs in pollutant reduction.

8CM.7

Airborne Measurements of Particle Size Distribution in Coal Power Plant Emissions Exhausted through Cooling Towers. JAN HOVORKA, Jaroslav Schwarz, Miroslav Klán, Filip Kozbrzek, Petr Marecek, *Charles University*

At nowadays, majority of coal-fired power plants in the EU pipe flue gas directly into natural-draft cooling towers to disperse particulate and gaseous pollutants. In cooling towers, the emissions are mixed with hot air and water vapor, receive intensified lift and also interact with droplets of large vapour plumes formed above the towers. While interaction between the plume droplets and SO₂ is well described, there was a very limited information on plume droplets-particulate matter interaction though the imminent importance of such a strong anthropogenic aerosol source. Therefore, airborne aerosol measurements were conducted in-and-off the vapour plumes above cooling towers of the Chvaletice coal-fired power station in Czechia. Spatial distribution and aerosol size spectra were determined by optical and aerodynamic particle sizers and a nanoscan spectrometer carried by an unmanned airship. An effective updraft of primary aerosol particles to the heights of 600m was confirmed. Measurement of mass and size distributions of supermicrone particles reveals horizontally narrow pollutant plumes enriched with PM_{2.5} up to 300 micrograms per cubic meter. Measurements of submicrone and ultrafine size spectra reveals dominant mode in 65 nm, reaching maximum number concentration about 10⁵ per cubic centimeter. Both findings indicate intensive post-injection cloud-processing of primary aerosol particles. The study is supported by the Technology Agency of the Czech Republic (TH02030238), the Czech Science Foundation (P503/12/G147) and the Sev.en Energy AG.

8IM.1

Towards More Accurate Particulate Organic Nitrate Quantification through Aerosol Mass Spectrometry. Frans Graeffe, Liine Heikkinen, LEAH WILLIAMS, Jean-Eudes Petit, Athina-Cerise Kalogridis, Andrew Lambe, Evelyn Freney, Philip Croteau, John Jayne, Manjula Canagaratna, Mikael Ehn, Olivier Favez, Alexandre Albinet, *University of Helsinki*

A large fraction of particulate organic nitrates (pON) arise from reactions involving volatile organic compounds (VOC) and nitrate radicals (NO_3) contributing significantly to tropospheric particulate matter. However, their quantification remains challenging. Previous studies with Aerosol Mass Spectrometers (AMS) show that the fragmentation patterns of inorganic ammonium nitrate and pON significantly differ from each other resulting in a clear contrast in the ratio between the major nitrate fragments, i.e., the $\text{NO}^+/\text{NO}_2^+$ ratio. Detection of pONs leads to larger $\text{NO}^+/\text{NO}_2^+$ values, but with high variability depending on the pON precursors. Additional uncertainty is also introduced while performing unit mass resolution (UMR) analysis as an organic ion fragment (CH_2O^+) is typically present at the same unit mass as NO^+ . Underestimation of this organic fragment can lead to significant overestimation of pON. As part of the Aerosol Chemical Monitor Calibration Centre (ACMCC) pON experiment, we generated pON via NO_3 oxidation of four different VOCs (limonene, β -pinene, guaiaicol, and acenaphthylene) in a Potential Aerosol Mass (PAM) oxidation flow reactor. The pON were detected with a High Resolution (HR) AMS equipped with a Long Time-of-Flight chamber facilitating a mass resolution approaching 8000 $M/\Delta M$, further enabling separation of nitrogen containing peaks in the mass spectrum. We observed precursor-dependent differences in the nitrate loading when comparing UMR and HR results mainly linked to CH_2O^+ underestimation with the default AMS fragmentation table. Here we present a modified fragmentation table with the goal of providing more accurate pON quantification in ambient air via UMR aerosol mass spectrometry such as Aerosol Chemical Speciation Monitor (ACSM). We also compare the abundance of other nitrogen-containing HR-AMS ion signals (e.g. combinations of carbon/hydrogen/nitrogen and carbon/hydrogen/nitrogen/oxygen atoms) obtained for the different pON types.

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8IM.2

A New Method to Quantify Mineral Dust, Sea Salt, Biomass Burning, and Other Aerosol Species from Aircraft Platforms using Single Particle Mass Spectrometry. KARL D. FROYD, Daniel Murphy, Charles Brock, Pedro Campuzano-Jost, Jack Dibb, Jose-Luis Jimenez, Agnieszka Kupc, Ann M. Middlebrook, Gregory Schill, Kenneth Thornhill, Christina Williamson, James Wilson, Luke Ziemba, *NOAA ESRL and CIRES*

Single-particle mass spectrometer (SPMS) instruments characterize the composition of individual aerosol particles in real time. Their high sensitivity to a wide variety of aerosol species, size-resolved capability, and ability to characterize internally and externally mixed aerosol species make SPMS instruments well suited to airborne studies of atmospheric aerosol composition. However, quantitative measurements using SPMS systems alone are inherently problematic. We present a new method that combines single-particle composition from the NOAA Particle Analysis by Laser Mass Spectrometry (PALMS) instrument with independently measured quantitative particle size distributions to determine absolute number, surface area, volume, and mass concentrations of mineral dust, biomass burning, sea salt, and other climate-relevant atmospheric particle types, with fast time response applicable to aircraft sampling. A statistical error analysis indicates that particle type concentrations can be determined for abundances above $\sim 10 \text{ ng m}^{-3}$ with sample times of only a few minutes. Rare particle types require longer sampling times. We also determine absolute mass concentrations of aerosol sub-components like sulfate or organic material within a particle class or across several classes. We summarize the principal sampling considerations and measurement criteria for deriving particle type concentrations from PALMS and other SPMS instruments, and we conclude with general recommendations for implementing the method in airborne composition studies. The wealth of information afforded by composition-resolved size distributions for all major aerosol types represents a new and powerful tool to characterize tropospheric and stratospheric aerosol properties in a quantitative fashion.

8IM.3

A New Method for Robust, Moderate-Cost Measurement of Oxygen, Carbon, and Sulfur Content of Organic Compounds and Mixtures. James Hurley, Nathan Kreisberg, Braden Stump, Patricia Keady, Susanne Hering, GABRIEL ISAACMAN-VANWERTZ, *Virginia Tech*

Health and climate impacts of aerosols depend on their composition. In particular, oxygen content controls the tendency of particles to form clouds, may drive adverse health effects, and provides insight into atmospheric oxidation processes. However, current methods to measure particle composition either rely on filter collection with low time resolution, or advanced mass spectrometers operated by highly-trained on-site personnel. We are developing an instrument for the time-resolved, in-situ measurement of aerosol organic carbon and its oxygen-to-carbon ratio, as well as aerosol sulfur. The approach is semi-continuous system, with concentrated particle collection coupled to commonly used gas analyzers, namely flame ionization (FID), flame photometric (FPD) and non-dispersive infrared (NDIR) absorption based detection of CO₂. We demonstrate that the average per-carbon-atom response generated by an FID is proportional to the oxygen content of an analyte. We quantify this relationship by directly measuring carbon dioxide produced in FID for ~100 individual atmospherically-relevant analytes. With this data, we are able to estimate oxygen-to-carbon ratios to within ~0.1 across the range of 0 to 1, and this relationship is shown to be valid for simple multi-component mixtures. FPD detection of sulfur within the same flame is shown to additionally provide quantification of inorganic and organic sulfur-containing compounds. We demonstrate the coupling of this detector train to online particle collection and stepped thermal desorption, providing the basis of an instrument that will enable remote, autonomous, and easy-to-calibrate measurements of particle composition (C, O, and S content) and particle volatility. Sensitivity of this approach is expected to allow measurements of the concentration and O:C of ambient organic aerosols at levels as low as ~1 µg/m³ with hourly time resolution.

8IM.4

Intercomparison of AMS and ACSM Measurements for Particulate Organic Nitrates (pON). ATHINA-CERISE KALOGRIDIS, Jean-Eudes Petit, Alexandre Albinet, Andrew Lambe, Liine Heikkinen, Frans Graeffe, Manuela Cirtog, James Allan, Zainab Bibi, Tanguy Amodeo, Nicolas Karoski, Laurent Meunier, Valerie Gros, Mikael Ehn, Tuija Jokinen, Minna Aurela, Marek Maasikmets, Axel C. Eriksson, Erik Ahlberg, Evelyn Freney, Konstantinos Eleftheriadis, MariCruz Minguillon, Leah Williams, Olivier Favez, et al., *NCSR Demokritos*

Particulate organic nitrates (pON) are important atmospheric species that are formed through the reactions of volatile organic compounds (VOCs) with atmospheric oxidants (OH/NO₃ radicals) and NO_x. They may account for a considerable fraction of fine particulate matter (PM_{2.5}) but their concentrations, sources and formation processes remain nearly unexplored aspects of atmospheric chemistry. Recently, a methodology based on time-of-flight aerosol mass spectrometer (ToF-AMS) measurements of NO⁺ and NO₂⁺ fragments of nitrate aerosol has been proposed to distinguish between inorganic nitrates and pON. However, this methodology has not been applied to quadrupole or time-of-flight Aerosol Chemical Speciation Monitors (Q-ACSM/ToF-ACSM) or to anthropogenic pON. In the present study, the response of 8 different ACSM, and 1 Long-ToF-AMS, instruments to pON was explored through a unique experimental setup under controlled conditions at the Aerosol Chemical Monitor Calibration Centre (ACMCC). pON were generated in a Potential Aerosol Mass (PAM) oxidation flow reactor from the reaction of NO₃ radical with single VOC precursors, two biogenic (limonene and β -pinene) and two anthropogenic (acenaphthylene and guaiacol). The results of this intercomparison will be presented, with a focus on variations in the mass spectra of pON (NO⁺/NO₂⁺, organics fragments and organic-to-nitrate ratios) as a function of: (1) instrumental configuration (AMS vs ACSM, Q-ACSM vs ToF-ACSM, standard vs capture vaporizers) (2) pON precursor (3) particle size and (4) particle mass concentration. Possible improvements of the default fragmentation table used to calculate the contributions to the signal for organic and nitrates will be proposed in order to account for interfering signals from other species. The impact of the observed variabilities on the NO⁺/NO₂⁺ methodology will also be investigated.

8IM.5

A Novel High-Resolution Ion Mobility Drift Tube with Diffusion Auto-correction. XI CHEN, Carlos Larriba-Andaluz, IUPUI

Ion Mobility Spectrometers (IMS) are becoming the standard equipment to measure nanoparticle distributions due to their simplicity, reproducibility, and portability. IMS separates nanoparticles through the particle's electrical mobility Z_p – the drift velocity of the particle divided by the electric field driving the movement-, and which is directly related to the size and charge of the entity as well as to the property of the gases. Despite the tremendous success of the differential mobility analyzer-condensation nucleus counter combination (DMA-CPC), there are a number of improvements which could be implemented in ion mobility technology to advance its use not only in aerosol science, but in biomolecular characterization and materials characterization. While one can improve resolution through geometric or external controls, this normally leads to poor signal and sensitivity due to loss of analytes through diffusion. The underlying problem with existing systems therefore arises from the inability to be able to control the diffusion broadening of the analytes that inevitably occurs in the detection cell of choice. Moreover, the resolution of existing devices is not mobility dependent which makes resolution at larger sizes insufficient. Accordingly, there is an urgent need to develop an instrument that can control the diffusion broadening of the signal and with resolution that scales with inverse mobility. Similarly, Scanning Mobility Particle Sizers (SMPS) typically require several minutes to complete voltage scans, and even in faster scanning instruments, particles of different sizes are sampled at different times. This limits information that can be obtained when aerosols are varying rapidly, such as can occur during sampling with an aircraft, near roadways, or from a combustion engine. Further, DMAs require the use of high sheath flow rates, and as such, require modest to high flowrate pumps which must remain stable during operation.

Here we show experimental evidence of a novel Drift Tube Ion Mobility Spectrometer working at atmospheric pressure which achieves resolutions of 100 ($Z/\Delta Z \sim 100$) for particle sizes between 0-30nm obtaining signals in a matter of milliseconds to seconds. We have accomplished this by applying linearly varying electric fields that control diffusion broadening and which allow the pulsing time to be large enough to allow large particle sizes through the pulsing gate. The resolution allows excellent separation between ions and nanoparticles while being able to monitor rapidly varying aerosols quite easily. The length of the tube is approximately 20cm (but can be reduced to 10cm with little to no consequences) and is quite simple and robust, e.g. it does not require polishing electrodes and does not require a very stable sheath flow to operate. Among the different test carried out, we have tested a mixture of 4 different tetraalkylammonium salts ranging from tetrabutylammonium to tetraheptylammonium bromide showing full separation on monomers dimers and trimers, something not possible on regular Differential Mobility Analyzers.

8IM.6

Quantifying Errors in Aerosol Mixing State Metrics due to Limited Particle Sample Size. Jessica Gasparik, NICOLE RIEMER, Matthew West, Qing Ye, Ryan Sullivan, Albert Presto, *University of Illinois at Urbana-Champaign*

Atmospheric aerosols are evolving mixtures of different chemical species. The term "aerosol mixing state" is commonly used to describe how different chemical species are distributed throughout a particle population. A population is "fully internally mixed" if each individual particle consists of same species mixtures, whereas it is "fully externally mixed" if each particle only contains one species. Mixing state matters for climate-relevant aerosol properties, such as the particles' propensity to form cloud droplets or the aerosol optical properties.

The mixing state metric χ quantifies the degree of internal or external mixing and can be calculated based on the particles' species mass fractions. Several field studies have used this metric to quantify mixing states for different ambient environments using sophisticated single-particle measurement techniques. Inherent to these methods is that a finite number of particles is used to estimate the mixing state metric, ranging from a few hundred to several thousand particles.

This study evaluates the error that is introduced in calculating χ due to a limited particle sample size. We used the particle-resolved model PartMC-MOSAIC to generate a scenario library that encompasses a large number of reference particle populations and that represents a wide range of mixing states. We stochastically sub-sampled these particle populations using sample sizes of 10 to 10,000 particles and recalculated χ based on the sub-samples.

The errors generated in χ from limited sample sizes were greater for external mixtures (maximum error of 324% for 10-particle sample), indicating that these mixtures require larger particle sample sizes to accurately represent the mixing state. Mean errors decrease for larger sample sizes, ranging from 76% to 3% for 10 and 10,000 particle samples, respectively. The finite sample size further leads to a consistent overestimation of χ . These findings are experimentally confirmed using SP-AMS measurement data from the Pittsburgh area.

8IM.7**Probing the Phase State and Viscosities of Sub-micron Organic Aerosols in Controlled Environmental Conditions.**

Noopur Sharma, KUO-PIN TSENG, Libor Kovarik, Swarup China, *Pacific Northwest National Laboratory*

Organic aerosols exhibit variability in their phase state and viscosity based on their material composition and the environmental conditions (like temperature and relative humidity). Viscosity of the organic aerosols influences particle growth rate, diffusivity, chemical reactivity, mixing state, and impacts the long-range transport of pollutants. Therefore, investigating the evolution of phase state/viscosity of organic aerosol or organic material with changing environmental factors is critically important. Currently available viscosity measurement techniques cater particle sizes greater than 20 μm , whereas atmospheric aerosols span submicron size ranges, which emphasizes the need of developing new apparatus for characterizing material properties of individual organic particles of atmospherically relevant size range while controlling the temperature and relative humidity.

In this study we present a novel technique combining Environmental Scanning Electron Microscopy (ESEM) with custom made environmental cell to allow tilted viewing of the sample while controlling the environmental conditions (relative humidity and temperature). Imaging particles in tilted view enables distinguishing particles based on their deformability when impacted on substrate during sample collection. Deformability of a particle is directly linked to the viscosity or phase state of its constituting material. Tilted imaging and ESEM together enabled us to investigate viscosity/phase state of various organic aerosols at given set of environmental conditions. Here, we discuss the principle and design of the novel set-up, present the results from the water uptake experiments, and report the phase transformation and hygroscopic growth factors of standard atmospherically relevant organics and ambient organic aerosol mixtures as a function of relative humidity and temperature. In next phase of development, we plan to introduce physical poking of the individual particles with micro-manipulator to obtain an estimate of their viscosities/phase states via poke-flow technique in ESEM.

8NM.1**Electroluminescence Induced by Electric Current through Defects of Cubic Magnesium Oxide Nanoparticles Synthesized by Self-Combustion Method.** CHANGHYUK KIM, Peter Pikhitsa, Sukbyung Chae, Kyungil Cho, Mansoo Choi, *Pusan National University*

Magnesium oxide (MgO) generally has a wide bandgap and no electrical conductivity. However, MgO nanoparticles synthesized through an aerosol method showed electrical conductivity due to the intrinsic defects built in the nanoparticles by the rapid synthesis in the air. Previously, it was reported that the intrinsic defects tuned the optical properties of MgO nanoparticles such as cathodoluminescence and photoluminescence (CL and PL), which were not observed from the commercial ones (Sigma-Aldrich Co.). In this study, an electroluminescence (EL) induced by the electric current through the intrinsic defects was observed at room temperature. The MgO nanoparticles were synthesized by the self-combustion of Mg chip in the air. The nanoparticles had cubic shapes and high purity, which were characterized by scanning electron microscope (SEM) and x-ray diffraction (XRD), respectively. The electrical conductivity was observed by electron beam absorbed current (EBAC). The EBAC images showed that the electrons emitted from the electron beam of SEM migrated through the edges of the contacting cubic MgO nanoparticles. When the MgO nanoparticles were sandwiched by electrodes and applied with voltage, the electrons migrating through the edges excited nitrogen (N_2) molecules around, thus showing the EL in the ultraviolet and visible range due to the micro N_2 discharge. These electroluminescence was not observed from the commercial MgO nanoparticles (Sigma-Aldrich), which also did not show the CL and PL before. Due to the defect-induced novel properties, the MgO nanoparticles with defects synthesized by the aerosol process are expected to apply for nanooptics, oxide electronics, gas adsorbents, etc.

8NM.2

A Numerical Model to Predict the Morphology of Particle Synthesized via Spray Pyrolysis. SUKRANT DHAWAN, Pratim Biswas, *Washington University in St Louis*

Spray pyrolysis is an aerosol process widely used for the continuous synthesis of nanoparticles. A precursor solution is usually sprayed into a carrier gas in the form of small droplets. Due to the high temperature of the surrounding gas, the solvent is vaporized, and a concentration gradient of the solute results inside the droplet. The solute gets precipitated and decomposed within the droplet to form particles. Particles with several different morphologies, such as solid and hollow shell, have been produced by spray pyrolysis process. The properties (chemical, electronic, optical) of the particles, and hence their application strongly depends on their composition, size, and morphology. Therefore, it is crucial to understand the different dynamic processes taking place in a droplet, in order to have better and more precise control on the morphology of the synthesized particles via spray pyrolysis. While several models have been developed in the past to predict the particle morphology, these models are missing the whole picture as they do not account for intradroplet reactions, formation, growth, and sintering of particles within the droplet.

In this presentation, a generalized droplet model of coupled heat and mass transfer developed to study the particle formation and predict the final morphology of particle synthesized via spray pyrolysis process will be discussed. The developed model accounts for different dynamic processes taking place during spray pyrolysis, such as droplet evaporation, solute diffusion inside droplet, reaction, and precipitation. The effect of different operating conditions and precursor properties, which influence the morphology of particles will be discussed. The model equations are further cast into dimensionless form for generalization, and the effects of governing dimensionless groups on the particle morphology are evaluated by performing a sensitivity analysis.

8NM.3

One-step Gas-phase Synthesis of Core-shell Nanoparticles via Surface Segregation. NAMSOON EOM, Markus Snellman, Martin Ek, Maria Messing, Knut Deppert, *Lund University*

A great amount of research effort has been devoted to the production of core-shell nanoparticles for applications in various fields including biomedical imaging, catalysis, and plasmonics. Such attention to core-shell nanoparticles arise from the fact that they can exhibit enhanced physical and/or chemical properties. Furthermore, core-shell particles with distinctly new properties compared to those of the constituent materials can be designed by tuning, for example, their size, shell thickness, and structure [1, 2].

Although chemical synthesis techniques are currently the most popular methods for fabricating core-shell nanoparticles, interface and surface contaminations are often an unavoidable issue in the solution-based approaches. Aerosol based methods are cleaner alternatives and have been used to produce core-shell nanoparticles [3-6]. Here we present aerosol core-shell nanoparticles generated via spark discharge generation (SDG) [7]. Cu-Ag core shell nanoparticles were fabricated via surface segregation using SDG accompanied by sintering directly in the gas phase. The surface segregation employed in this method refers to the phenomenon of the enrichment of one component of a mixture in the surface region and is attributed to the interplay between the atomic radii, cohesive energy, and surface energy of the core and shell materials [8].

Depending on the sintering temperature, the SDG-generated nanoparticles form Janus-like or core-shell structures. The morphology, crystallinity, and composition of the SDG-generated bimetallic nanoparticles were investigated by scanning electron microscopy, high-resolution transmission electron microscopy, and energy-dispersive X-ray spectroscopy. Molecular dynamics simulations were carried out to investigate the structural evolution of Cu-Ag nanoparticles during heating and cooling processes corresponding to the sintering. This appealingly simple one-step gas-phase synthesis method presented here can be employed for other bimetallic systems.

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8NM.4

Analysis of Si Nanoparticle Growth in Low Pressure Non-thermal Plasmas and Plasma Afterglows via Differential Mobility Analysis and Monte Carlo Simulations. XIAOSHUANG CHEN, Takafumi Seto, Uwe R. Kortshagen, Christopher Hogan Jr., *University of Minnesota*

Low pressure (< 10 Torr) non-thermal plasma flow tube reactors are frequently utilized for the production of crystalline group 14 semiconductor nanocrystals from vapor phase precursors. Although it is desirable to monitor reactor output and particle growth dynamics, online size distribution determination of non-thermal plasma synthesized nanoparticles is a challenge; the sub-atmospheric operating pressure of most non-thermal plasmas makes it extremely difficult to couple traditional atmospheric pressure aerosol mobility instrumentation to reactors.

In this study, we applied a low pressure differential mobility analyzer (LPDMA) to examine the mobility distributions of Si nanoparticles synthesized via silane reaction in a radiofrequency Argon plasma at 2 Torr. We experimentally evaluated the transfer function of the LPDMA and developed a data inversion routine to determine the collision cross section distribution functions of the charged particles exiting the plasma. The collision cross section is the most direct measure of particle size in the free molecular regime, hence we elected to use it as the measure of nanoparticle size in this study. Inverted collision cross section distribution functions agree well with those inferred from TEM images of particles.

Interestingly, we were able to detect both negatively charged and positively charged particles at the plasma reactor outlet. Particles are expected to be unipolarly charged in the plasma volume, mainly because of the large mass and mobility differences between electrons and Argon ions. We hence subsequently studied nanoparticle aggregation in the afterglow region of the plasma reactor by varying the allowable time for nanoparticle growth between the plasma reactor and the LPDMA, showing that nanoparticles rapidly aggregate after exiting the plasma. Measurements of size distribution evolution in the afterglow were compared to a constant-number Monte Carlo simulation accounting for ion and electron losses, particle-ion and particle-electron collisions, charge ejection from high charged particles, and particle-particle collisions.

8NM.5

A Versatile Aerosol-based Technique to Deposit Nanoparticle Thin Films from Colloidal Solutions. SHALINEE KAVADIYA, Jonathan Bryan, Yuji Okamoto, Peter Firth, Hussain Saddam, Zachary Holman, *Arizona State University*

Nanoparticles have revolutionized many industries in the past few decades because of their small size and high surface area to volume ratio. Many of the fields, from healthcare to food manufacturing and energy conversion and storage, require nanoparticles to be deposited as a functional thin film that maintains or even enhance the functional properties of the material. Nanoparticles are conventionally synthesized using wet-chemistry methods, resulting in a colloidal solution or dry powders. A variety of techniques are currently present to deposit these particles on a surface, namely, spin coating, spray technique, ink-jet printing, evaporation, plasma-based printing, sputtering, etc. However, these techniques are either not versatile or do not have precise control.

Therefore, the aim of this work is to develop a versatile technique, Aerosol Impaction-Driven Assembly (AIDA) to deposit a nanoparticle thin film on any kind of substrate with control over the film properties. The technique involves a two-step spraying process. In the first step, a colloidal solution of nanoparticles is sprayed through an ultrasonic atomizer nozzle in a low-pressure chamber (1-50 Torr) generating droplets containing nanoparticles. The droplets are carried with a carrier gas and solvent from the droplets is evaporated. In the second step, the nanoparticles are passed through a fine orifice nozzle along with a carrier gas into a deposition chamber with much lower pressure (0.1-5 Torr). The large pressure ratio (10-fold) accelerates the nanoparticles to supersonic velocity, creating a spray of nanoparticles. The low pressure downstream of the nozzle reduces the drag force on the nanoparticles and enables them to deviate from the gas stream and impact on a substrate, forming a thin film rather than flowing away along with the carrier gas. Using this technique, a thin film can be deposited conformally on any type of substrate, from planar Si wafer to a textured wafer. Dry deposition of 50 nm silver particles is achieved, and a uniform coating of a thin film is in progress.

The presentation will discuss the mechanism, challenges, and applications of this technique.

8NM.6

Optical Monitoring of Aerosol Thermal Processing. JAMES RADNEY, Christopher Zangmeister, *National Institute of Standards and Technology*

The thermal processing (e.g. chemical reduction, particle dehydration, thermal decomposition, etc.) of nanoparticles using furnace reactors has seen significant use due to the simplicity and scalability of the process. The ability to control temperature and reaction conditions enables a wide array of chemical and thermal process to occur, enabling the development of new nanomaterials. A major challenge is the measurement of aerosol chemical reactions in real-time, in-situ. Here we introduce and demonstrate a new in-situ method that measures aerosol mass and spectroscopic changes as a function of reaction temperature. Two systems were investigated: the evolution of CuO from CuSO₄·5H₂O and the reduction of graphene oxide to graphene in a furnace reactor. The physical properties of the particles (size and mass) were characterized utilizing a combination of multiple differential mobility analyzers (DMAs) and an aerosol particle mass analyzer (APM) while spectroscopic (extinction and absorption) changes were probed using 2- λ cavity ring-down and photoacoustic spectroscopies, respectively. This combination of optical measurements allows for determination of the absorption Ångström exponent and co-albedo at 2- λ which can be used as proxies for particle color.

8NM.7

Observing, Predicting and Controlling Crystalline and Amorphous Particle Formation in Evaporating Aqueous Aerosol Droplets. JONATHAN P. REID, Florence Gregson, Rachael E.H. Miles, Jim Walker, Daniel Hardy, Justice Archer, Joshua Robinson, Royall Patrick, *University of Bristol*

The evaporation of aqueous aerosol droplets to form dry crystalline or amorphous particles is a fundamental process that is important for understanding the phase of atmospheric particles and is exploited in industrial processes such as spray drying. The phase, composition and heterogeneity of the final particle is dependent on the drying conditions (for example, relative humidity and temperature) and the presence of additives (for example, the presence of surfactants and co-solvents). Further, as a particle loses solvent and decreases in size, the viscosity and diffusivity of the different chemical components can vary over many orders of magnitude, slowing the loss of water and leading to amorphous particles that release moisture over very long-time frames. Using experimental tools for probing the rapid drying dynamics of single particles, new insights can be gained into the microphysical processes that determine the phase and microstructure of the final particle. Specifically, we will report measurements using an electrodynamic balance and using a falling droplet instrument, providing access to time-resolutions spanning from 10 μ s to hours and allowing direct measurements of the evaporation kinetics, transient morphologies from high time-resolution imaging, and final particle morphologies from scanning electron microscopy. From these experiments, we will contrast the well-defined crystallization time and final morphologies of the binary salt sodium chloride with the behavior of alkali metal nitrates solution droplets, which often form amorphous particles. By incorporating long-chain alcohols, we will demonstrate control over the crystallization time and final particle size during droplet drying. We will also explore the different stages of drying of aqueous saccharide solution droplets, contrasting the rapid initial loss of water with the much longer stage of drying as the particle becomes increasingly viscous, reporting measurements of the evolving mass over many hours.

9AC.2

Simulation of SOA Formation from the Photooxidation of Gasoline in the Presence of NO_x and Electrolytic Inorganic Aerosol. MYOSEON JANG, Chufan Zhou, Zechen Yu, Sanghee Han, *University of Florida*

The prediction of secondary organic aerosol (SOA) mass is complex due to variation and complexity in the atmospheric process of hydrocarbons under varying NO_x, SO₂, sunlight, humidity and temperature in ambient environments. Our laboratory's recent efforts have improved the state-of-the-science-art via the development of the UNified Partitioning-Aerosol phase Reaction (UNIPAR) model, which features the product stoichiometric coefficients (51 lumping groups) based on volatility (6 groups) and reactivity (8 groups) to consider their emerging chemistry in the aerosol phase. In the model, Glyoxal, methylglyoxal, and IEPOX, which are known to significantly contribute to SOA formation, are explicitly treated. The preexisting UNIPAR vastly improves the accuracy of SOA mass prediction for each precursor owing to the stoichiometric coefficient array set that is dynamically generated under varying NO_x and aging conditions but specific to each precursor. The SOA model, however, needs simplification and unification to treat a variety of precursor hydrocarbons appeared in ambient air. In this study, UNIPAR is extended to the simulation of gasoline SOA that is attributed to various hydrocarbons to mimic SOA formation under urban environments. In UNIPAR extension, the model parameters, linked to partitioning of oxygenated organic species in multiphase and their reaction rate constants in aerosol (i.e. oligomerization in organic phase, acid-catalyzed reactions in inorganic aqueous phase, and organosulfate formation), are cohesive for various aromatic precursors. The dynamic stoichiometric coefficient array set, which changes by NO_x and aging conditions, is also cohesive to various aromatic precursors in the extended UNIPAR. The consumption of aromatic precursors in gasoline is predicted by using Carbon Bond Mechanism (CB6) and integrated with UNIPAR to predict SOA mass. The feasibility of UNIPAR is demonstrated with chamber data (UF-APHOR), which produce SOA from the photooxidation of gasoline in the presence of electrolytic inorganic aerosol and NO_x.

9AC.3

Recent Declines in Water Uptake and Acidity of Inorganic Aerosols during Beijing Winter Haze Events. SHAOJIE SONG, *Harvard University*

In recent years, aggressive air pollution mitigation measures in China have resulted in considerable changes in gas and aerosol chemical compositions. However, the responses of aerosol water uptake and acidity, two parameters pivotal to the formation of severe northern China winter haze events, to such changes remain uninvestigated. Here, we performed thermodynamic equilibrium modeling using gas and aerosol composition and meteorological data observed during three winter seasons in urban Beijing, and quantified the changes in the mass growth factor and pH of inorganic aerosols. We found, from the winter haze condition in 2014/2015 to that in 2017/2018, that the mass growth factor decreased by about 10% due to changes in aerosol chemical compositions (more nitrate and less sulfate and chloride) and that pH increased by about 0.2 unit owing to rising excess ammonia. The buffer equation for the gas-particle system was derived for the first time and was very helpful to conceptually understand the sensitivity of aerosol pH to meteorological variables and chemical compositions. These new insights had implications for evaluating the potential chemical feedbacks in secondary aerosol production and the role ammonia played in haze formation.

9AC.4

Emergence of a New Chemical Regime: Growing Abundance of Water Soluble Organics in Cloud Water Associated with a Growing Ion Imbalance. CHRISTOPHER LAWRENCE, Sara Lance, James Schwab, James Dukett, Kevin Civerolo, Oliver Rattigan, Dan Kelting, Elizabeth Yerger, Hunter Favreau, Paul Casson, Richard Brandt, *University at Albany, SUNY*

Long-term reductions in anthropogenic sulfate in the eastern U.S. have been captured by observations spanning several decades across New York State, including cloud water composition measurements at Whiteface Mountain (WFM). These observations reflect one of the major goals of the Clean Air Act: dramatic reductions in sulfuric acid deposition. Concomitant long-term reductions in nitrate and ammonium have also been recorded, associated with reduced particulate mass loadings. Altogether, these outcomes are considered one of the greatest success stories in the history of U.S. air pollution regulation.

Due to the historical impetus for cloud water monitoring in the eastern U.S., measurements at WFM began with inorganic ion speciation, which has continued largely unchanged to the present day. Measurements of Water Soluble Organic Carbon (WSOC) were added in 2009. In the past decade cloud water samples have become increasingly anion deficient, leading to a growing number of samples considered "invalid" due to ion imbalance. While most published literature on cloud water composition does not include "invalid" samples, in the present day "invalid" samples outnumber "valid" samples. The growing ion imbalance suggests that there is a growing abundance of anions that are not detected with the traditional suite of measurements. When choosing not to apply these ion balance criteria in the data analysis, a striking increase in WSOC emerges over the past decade. A growing abundance of ammonium in cloud water has also reached a new milestone, surpassing both sulfate and nitrate combined. Thus, while the acidity of cloud water has decreased dramatically, these observed changes in cloud water composition suggest that we are entering a new chemical regime in the northeastern U.S., which is not necessarily "clean".

We report on the re-evaluation of these long-term trends and describe the addition of an important constituent to our cloud water monitoring efforts: organic acids.

9AC.5

IEPOX-Derived Organosulfates Contribute a Significant Portion of the Aerosol Mass Spectral Tracer Ion of IEPOX-derived SOA and Its Implications. YUE ZHANG, Yuzhi Chen, Manjula Canagaratna, Sri Hapsari Budisulistiorini, Tianqu Cui, Zhenfa Zhang, Avram Gold, John Jayne, Douglas Worsnop, Barbara Turpin, Jason Surratt, *Univ. of North Carolina, Chapel Hill/Aerodyne Research, Inc.*

Isoprene-derived secondary organic aerosols (SOA), an important fraction of the global aerosol budget, often form through acid-catalyzed heterogeneous reactions of isoprene epoxydiols (IEPOX) onto acidified sulfate particles. An enhanced fraction of the $C_5H_6O^+$ ion ($f_{C_5H_6O}$), with a mass-to-charge (m/z) ratio of 82, is found to be present in aerosol mass spectra of IEPOX-derived SOA from both field and laboratory measurements and commonly identified as a tracer ion. The origin of the tracer ion remains uncertain due to the complex composition of IEPOX-derived SOA.

2-Methyltetrols and 2-methyltetrol organosulfates, the two groups of compounds that account for more than 90% of *trans*- β -IEPOX derived SOA, were atomized into the Aerodyne Aerosol Chemical Speciation Monitor (ACSM). The mass spectral data show that a large $f_{C_5H_6O}$ surprisingly appears in the mass spectrum of pure 2-methyltetrol organosulfates aerosols. Positive matrix factorization (PMF) was applied to the time-series data of IEPOX reacting with acidified ammonium sulfate particles in the UNC chamber to examine the time-dependent compositional changes of the SOA. PMF-derived factor was successfully resolved for 2-methyltetrol organosulfates in the aerosol phase, with a correlation factor greater than 0.9 when compared with pure standards and the particle into liquid sampler (PILS) coupled to hydrophilic interaction chromatography interfaced to electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (HILIC/ESI-HR-QTOFMS). Multilinear engine (ME-2) was used to source apportion the organosulfate fractions from field data obtained from Atlanta, GA, and Look Rock, TN. Results suggest a higher than expected organosulfate mass fraction present in ambient IEPOX-derived SOA. Our findings indicate that the tracer ion at m/z 82 for IEPOX-derived SOA measured during field and laboratory studies is likely a fragmentation product of organosulfates that are prevalent in ambient IEPOX-derived SOA. Higher organosulfate concentrations may lead to important changes in the aerosol physical properties and chemical reactivity due to their unique properties.

9AC.6

Combined Impacts of Acidity and Viscosity on the Formation of Inorganic-Organic Mixed Isoprene Epoxydiol (IEPOX)-Derived Aerosols. YUE ZHANG, Yuzhi Chen, Ziyang Lei, Nicole Olson, Matthieu Riva, Abigail Koss, Zhenfa Zhang, Avram Gold, John Jayne, Douglas Worsnop, Timothy Onasch, Barbara Turpin, Jesse Kroll, Andrew Ault, Jason Surratt, *University of North Carolina at Chapel Hill*

Acid-driven reactions are an important formation mechanism for atmospheric secondary organic aerosol (SOA). Isoprene-derived SOA is often formed through acid-driven reactive uptake of isoprene-derived epoxydiols (IEPOX) onto acidic sulfate particles. These multiphase processes convert a significant portion of the inorganic sulfate into organosulfates, during which changes in aerosol physicochemical properties have not been well characterized. This study systematically examines the phase state, acidity, and morphology of aerosol particles as IEPOX reacts with acidified ammonium sulfate particles.

Chamber studies show that heterogeneous reactions of IEPOX is accompanied by the rapid formation of IEPOX-derived SOA, but further IEPOX uptake is impeded by its reaction products, especially the organosulfates. To explain such phenomenon, a thermodynamic model and a viscosity model are combined to predict the drastic changes of aerosol viscosity and acidity during this process. Notably, the hydronium ion (H^+) aerosol concentration decreases nearly by 1.5 pH units, and viscosity increases by more than 7 orders of magnitude from the beginning of the reaction to the end. SOA converts into a core-shell morphology with inorganic components remaining in the core and the organic components in the shell. Initial IEPOX-to-inorganic sulfate ratios as well as aerosol acidity and viscosity play critical roles in the inhibition of additional multiphase chemical reactions of IEPOX, explaining the self-limiting effect of IEPOX-derived SOA formation. Drastic changes in aerosol acidity and viscosity result in significant changes in the physicochemical properties of aerosols, which in turn alters the chemical reactivity. Our findings reveal important interconnections between the physical and chemical properties of the aerosol particles that come from interactions of inorganic and organic components. These results have important implications for understanding isoprene-derived SOA formation and the interplay between multiphase chemical processes that ultimately control atmospheric SOA formation and its impact on climate, human health, and visibility.

9AC.7

Aerospec – An Online Platform for Analysis of Chemical Composition of Aerosols. HE JIAYANG, Gaurav Mahamuni, Jay Rutherford, Jiawei Zhang, Igor Novosselov, Edmund Seto, *University of Washington*

Chemical composition of ultrafine particulate matter (PM), such as emissions from combustion sources, is important in characterizing the health impact of an individual's exposure. Polycyclic aromatic hydrocarbons (PAHs) are a widespread class of environmental chemical pollutant found in combustion-generated PM. Monitoring of PAH compounds via analytical chemistry techniques presents difficulties due to the high cost of analysis. These PAHs have strong fluorescence signatures. Our web-based platform (AeroSpec) utilizes fluorescence spectroscopy analysis technique, i.e., excitation-emission matrix (EEM) and principal component analysis (PCA) to estimate PAH content of combustion generated aerosols. The EEM spectra can be uploaded through the web interface and compared with the spectra library developed based on the data from laboratory and real-world samples. The EEM spectra library contains sample data correlated with Gas Chromatography-Mass Spectrometry (GC-MS) data which enable comparison to spectra from known PAH and single source laboratory samples. The AeroSpec platform was tested for a variety of real-world samples including diesel exhaust, cookstove smoke, and cigarette smoke.

9AC.8

Observation on Chemical Characteristics of Airborne Particles in Xi'an, Inland China during Dust Storm Events with Implications for Heterogeneous Formation of Ammonium Nitrate and Enhancement of N-deposition. GEHUI WANG, Wu Can, Jianjun Li, Cong Cao, Jin Li, *East China Normal University*

To identify the sources and heterogeneous reactions of sulfate and nitrate with dust in the atmosphere, airborne particles in Xi'an, inland China during the spring of 2017 were collected and measured for chemical compositions, along with a laboratory simulation of the heterogeneous formation of ammonium nitrate on the dust surface. Our results showed that concentrations of Ca^{2+} , Na^{+} and Cl^{-} in the TSP samples were enhanced in the dust events, with the values of 41.8, 5.4 and 4.0 $\mu\text{g}/\text{m}^3$, respectively, while NO_3^{-} (7.1 $\mu\text{g}/\text{m}^3$) and NH_4^{+} (2.4 $\mu\text{g}/\text{m}^3$) remarkably decreased, compared to those in the non-dust periods. During the dust events NH_4^{+} correlated only with NO_3^{-} ($R^2=0.52$) and abundantly occurred in the coarse mode ($>2.1 \mu\text{m}$), in contrast to that in the non-dust periods, which well correlated with sulfate and nitrate and enriched in the fine mode (2.1 μm), suggesting that they were directly transported from the upwind Gobi Desert region. Our laboratory simulation results showed that during the long range transport hygroscopic salts in the Gobi dust such as mirabilite can absorb water vapor and form a liquid phase on the particle surface, then gaseous NH_3 and HNO_3 partition into the aqueous phase and form NH_4NO_3 , resulting in the strong correlation of NH_4^{+} with NO_3^{-} and their accumulation on dust particles. The dry deposition flux of total inorganic nitrogen ($\text{NH}_4^{+} + \text{NO}_3^{-}$) in Xi'an during the dust events was 1.28 $\text{mg}/\text{m}^2/\text{d}$ and 80% higher than that in the non-dust periods. Such a significant enhanced N-deposition is ascribed to the heterogeneous formation of NH_4NO_3 on the dust particle surface, which has been ignored and should be included in future model simulations.

9AC.9

Effects of Common Inorganic Salts on Aqueous Photochemistry of Secondary Organic Aerosol. ALEXANDRA KLODT, Dian Romonosky, Peng Lin, Julia Laskin, Alexander Laskin, Sergey Nizkorodov, *University of California, Irvine*

The mechanisms by which atmospheric salts change the aging of secondary organic aerosols (SOA) in cloud and fog waters are poorly understood. To address this, products of SOA aging were measured in aqueous solutions with cloud or fog water relevant concentrations of some common atmospheric salts or oxidants. The SOA was produced from a common monoterpene (α -pinene) and a common sesquiterpene (α -humulene) through ozonolysis in a flowtube. After the SOA was collected on filters, the water-soluble portion of the SOA was extracted from the filter into pure water or aqueous solutions containing dilute concentrations of H_2O_2 , NaNO_3 , or NH_4NO_3 . Aqueous samples were exposed to light in the actinic region for four hours (approximately equivalent to 64 hours in the atmosphere) or kept in the dark for four hours to simulate daytime or nighttime processing. Compositional changes were monitored by high-resolution electrospray ionization mass spectrometry at one-hour intervals, and the resultant spectra showed that the presence of salts preferentially removed higher molecular weight compounds with or without photolysis. This increased the volatility of the SOA as efficiently as or more efficiently than photolysis in pure water. This result could impact our understanding of SOA lifetimes and aging in dilute atmospheric waters such as cloud and fog waters.

9AC.10

Growth Mechanisms of Size-Selected Ammonium Sulfate Seed Particles by Monoterpene Ozonolysis. JUSTIN KRASNOMOWITZ, Michael J. Apsokardu, Devon Haugh, Michael Taylor, Murray Johnston, *University of Delaware*

Aitken mode particles (10-100 nm in diameter) often represent the largest number fraction of particles found in the ambient environment. Understanding the processes contributing to the growth of these particles is paramount to better predict formation of cloud condensation nuclei (CCN). Low volatility organic compounds formed through gas phase oxidation of biogenic volatile organic compounds (BVOCs) such as α -pinene and limonene with low volatility have been shown to be the major source of particle growth in this size range. We have studied particle growth as a function of seed particle size and gas-phase reactant mixing ratios for α -pinene ozonolysis using a flow tube reactor and kinetic modeling. Results with dry seed particles suggest a condensational growth mechanism with a yield of condensable organic molecules of 13% from the ozonolysis reaction (Krasnomowitz et al., AS&T 2019). This yield is somewhat higher than the yield of highly oxidized molecules (HOMs) in the gas phase determined by chemical ionization. There are several reasons why the yields of condensable molecules obtained from gas- and particle- phase measurements can be different. Currently, we are investigating the effects of relative humidity on the same system. Preliminary results show that under equivalent experimental conditions including relative humidity, deliquesced ammonium sulfate particles grow much faster than dry seed particles. This effect is observed exclusively for particles below about 50 nm in diameter. Molecular composition measurements of the grown particles show that deliquesced particles contain a larger fraction of oligomers than dry particles, suggesting that particle phase chemistry contributes to the enhanced growth. Kinetic modeling to explain the particle-phase chemistry will be presented as well as particle size measurements by SMPS, molecular composition by HR-ESI-MS and single particle elemental composition by NAMS. Additional experiments focused on growth by limonene ozonolysis are underway and also will be discussed.

9AC.11

Accelerated Reaction of Carbonyls in Aerosol Droplets Studied with Droplet Assisted Ionization. YAO ZHANG, Michael J. Apsokardu, Devan E. Kerecman, Murray Johnston, *University of Delaware*

Droplet assisted ionization (DAI) is a method developed in our laboratory for online analysis of aqueous droplets. This method is ideally suited for studying the kinetics of aerosol reactions. In the current work, we present a kinetic study of the reaction of Girard's T reagent (GT) with carbonyls in α -Pinene Secondary Organic Aerosol (SOA). This reaction proceeds very slowly in bulk solution, but quickly in aerosol droplets. The time dependence of the reaction was varied by changing the tube length, and therefore the droplet transit time, between the atomizer where droplets are initially formed and the mass spectrometer where the molecular products and reactants in the droplets are detected. The reaction rate constant was determined from the time dependence of product and reactant signal intensities assuming pseudo-first order kinetics. The activation energy associated with reaction acceleration was determined from the dependence of product and reactant signal intensities on the temperature of the DAI inlet. The results give insight into the mechanism of enhanced reactivity in aerosol droplets.

9AC.12

Elucidation of the Influence of Specific Meteorological Conditions on the Electrostatic Charging State of Ambient Aerosols by a Parallel Electrode Plate Device. RYOYA TABATA, Ayumi Iwata, Kentaro Fujioka, Tomoaki Okuda, *Keio University*

In recent years, the influence on health by fine aerosol particles such as PM_{2.5} has been concerned. Especially regarding the particle deposition in a human airway, some previous studies show that the deposition rate of charged particles to airway surface is several times higher than that of uncharged particles. However, little knowledge on the electrostatic charging state of atmospheric aerosols has been obtained so far. Therefore the electrostatic charging state of atmospheric aerosols has been measured since April 2017 using a parallel electrode plate device utilizing the principle of electric mobility. We call this device K-MACS (Keio-Measurement System of Aerosol Charging State). The flow path of K-MACS is divided into three, and when +1.5 kV is applied, uncharged particles come out from the middle exit. Therefore we compare the number concentration of particles coming out from the middle exit with that of the inlet and calculate the proportion of uncharged particles.

The results varied depending on the measurement day, and the proportion of uncharged particles was about 12-25%. By investigating the relationship between the electrostatic charging state and the meteorological condition at the time of measurement, there was a strong positive correlation between the proportion of uncharged particles and the volumetric humidity. To investigate the relationship between the proportion of uncharged particles and the volumetric humidity, we measured the electrostatic charging state while the volumetric humidity was manually changed. When a continuous measurement of the uncharged particles proportion was conducted at sunny weather condition, there was a strong positive correlation between the proportion of uncharged particles and the oxidant concentration. As a factor of correlation, we thought that secondary generated particles influenced the electrostatic charging state of ambient aerosols. Therefore, we simultaneously measured the electrostatic charged state, Aitken particles, and the atmospheric ion concentration.

9AC.13

Chemical Characterization of Secondary Organic Aerosol Formed from the Photoreactions of Guaiacyl Acetone in an Aqueous Particle Extract. WENQING JIANG, Richie Kaur, Martin Brüggemann, Hartmut Herrmann, Cort Anastasio, Qi Zhang, *University of California, Davis*

Guaiacyl acetone (GA) is a typical phenol emitted in significant quantities from biomass burning through lignin pyrolysis. With a high Henry's law constant, GA readily partitions into atmospheric aqueous phases, where it reacts to produce secondary organic aerosol (SOA). In addition to fog and cloud waters, these aqueous reactions can also take place in particle-bound water, which is ubiquitous and persistent in the atmosphere despite low liquid water contents. In addition, recent studies have shown the concentrations of some photooxidants in particle water to be higher than in fog waters (Kaur et al., ACPD, 2018). Also, the high concentrations of organics, salts and metals in particle water could affect aqueous photooxidation reactions. In this study, we use high resolution time-of-flight aerosol mass spectrometry (HR-ToF-AMS) and Orbitrap mass spectrometry coupled to liquid chromatography (LC-Orbitrap MS) to investigate the chemical composition of the SOA formed from photoreactions of GA in an aqueous extract of wintertime particulate matter (PM extract) collected in a residential area with significant wood burning. GA oligomers and their derivatives are observed in the irradiated GA-PM extract solution by LC-Orbitrap MS and AMS. The AMS analysis further shows that ion signals representative of GA oligomers (e.g., $C_{20}H_{22}O_6^+$ and $C_{18}H_{19}O_5^+$) increase at the beginning of irradiation and then decrease. It suggests that oligomerization of GA is more important early in the reactions, but fragmentation becomes more important in later periods. In addition, the nitrogen-to-carbon ratio of the GA-PM extract solution increases from 0.37 to 0.44, and the contribution of $C_xH_yN_p^+$ and $C_xH_yO_zN_p^+$ signals in the AMS mass spectra increases from 7.3% to 9.0% during irradiation, indicating the formation of N-containing organic compounds. A large number of N-containing compounds formed in the photooxidation of GA are identified by LC-Orbitrap MS.

9AC.14

Impact of Wildfire on Ambient Air Levels of Unsubstituted and Alkylated-PAHs in the Region of Oil Sands Exploitation and Bitumen Processing in Alberta, Canada. ANDRZEJ WNOROWSKI, Jean-Pierre Charland, *Environment and Climate Change Canada*

Characterization of air pollutants emitted during wildfires in the Athabasca Oil Sands Region is important for understanding their impact on human health and ecosystems and their combined effects with air pollutants emitted from oil sands related exploration and processing in the region. The burden of wildfire emissions on ambient air levels of alk-PAHs in the oil sands region is not fully understood, consequently comprehensive emission source apportionment, evaluation and control of the environmental risks are still incomplete. On May 15, 2011, a wildfire started in the Richardson Backcountry area (Alberta, Canada) and burned until the end of June, consuming 577,647 hectares of boreal forest (Canadian Wildland Fire Information System, 2018). This wildfire spread across the Athabasca region and came within 10 to 30 km of the ambient air monitoring stations in the oil sands region. This resulted in the detection of substantially higher levels of unsubstituted and alkylated-PAHs (PACs) during this fire episode (May 15 to June 30, 2011).

The measured PAC levels differed amongst the three regional air monitoring stations in relation to distance from the wildfire and oil sands industrial locations. In addition, we observed an unexpected high contribution of alkylated-PAHs which suggests that wildfire emissions in the oil sands region are unique and contribute notably to the overall annual burden of unsubstituted and alkylated-PAHs in ambient air. The study highlights the notable contribution of alkylated-PAHs that are not routinely monitored in air, and that wildfire emissions can be characteristic to the region where previously deposited or naturally present chemical species such as PACs can be released to air at high temperatures occurring during fires.

9AC.15

The Role of the Solvent Environment on Physical Properties in Secondary Organic Aerosol Mimicking Solutions. Rebecca Miller, Hannah Inman, Emmaline Longnecker, Lucy Metz, ANDREW BERKE, *Smith College*

Reactions between small dicarbonyl compounds and amines represent a useful model system for studying non-oxidative chemistry in secondary organic aerosols (SOAs). The chemical transformations that occur within the aqueous layer of a particle are mediated by the solvent environment surrounding those transformation reactions. Bulk-phase reactions of aerosol mimicking solutions offer insights into the role(s) of specific solute-solvent interactions, which have consequences for the production of light-absorbing compounds and aerosol physical properties. We seek to understand the role of small, oxidized solutes on these SOA-transforming chemical reactions.

Our research specifically focuses on understanding the effects of compounds containing alcohol, nitrile, or ketone functionality on the chemistry and physical properties of bulk-phase SOA-mimicking solutions that contain glyoxal and ammonium sulfate. Results will be presented for solution matrices that contain short-chain alcohols, diols, acetonitrile, and acetone. We study bulk solution properties, such as viscosity, and intermolecular interactions within the solvent matrix through infrared spectroscopy (IR-ATR). Perturbations to the solvent environment have wide-ranging effects on the reaction between glyoxal and ammonium sulfate and will be presented, including changes to solution viscosity as functions of species and concentration added. Applications of these bulk-phase studies to aerosol particles will be highlighted. System thermodynamics will also be discussed.

9AC.16**Assessing the Contribution of NO₃ Radical Chemistry to Nanoparticle Composition in the Boreal Atmosphere.**

DANIELLE C. DRAPER, Michael Lawler, Theo Kurten, James Smith, *University of California, Irvine*

Products consistent with NO₃ radical-initiated oxidation of monoterpenes have been observed in nanoparticles measured at the SMEAR II station in Hyytiälä, Finland, using the Thermal Desorption Chemical Ionization Mass Spectrometer (TDCIMS). Several organic nitrates, detected as molecular ions and as thermally decomposed fragments, displayed a striking diurnal profile, peaking at night and comprising a significant fraction of total compounds measured by the TDCIMS. These same ions have also been measured by the TDCIMS during monoterpene and NO_y-containing chamber experiments. Products identified are consistent with first-generation oxidation products, which are assumed to be semivolatile and thus surprising to contribute strongly to nanoparticle composition under ambient conditions. Observed time series are assessed with kinetics and partitioning modeling approaches, using vapor pressures estimated using the SIMPOL group contribution method, as well as using the quantum chemical software COSMOtherm to obtain closure between our measurements and known partitioning theory. This work adds to the growing body of literature that suggests NO₃ oxidation of monoterpenes is a strong contributor to SOA formation in forested environments. Furthermore, it emphasizes the potential importance of this chemistry in the growth of atmospheric nanoparticles.

9AC.17**Modeling Studies of Isoprene- and Monoterpene-derived Organic Nitrates in a Mixed Forest Environment and the Role of Deposition and Aerosol Multiphase Chemistry.**

ISAAC CANADA, Paul Shepson, Jonathan Slade, *University of California, San Diego*

Organic nitrates (RONO₂) produced during the oxidation of VOCs in the presence of nitrogen oxides (NO_x=NO+NO₂) limit ozone production by sequestering NO_x and contribute to secondary organic aerosol (SOA) formation. While forested environments represent the largest source of biogenic VOC emissions, and biogenic SOA is the most abundant source of OA in the atmosphere, the formation of biogenic-derived RONO₂ is poorly understood with sparse measurements. Here, we present modeling results of RONO₂ and compare to measured RONO₂ sampled in a mixed deciduous/coniferous forest in northern Michigan during the summer of 2016. During that study, concentrations of hydroxylated RONO₂ (HORONO₂) resulting from the oxidation of isoprene (IN) and monoterpenes (MTN) were quantified over multiple daily cycles. We apply a 0-D chemical kinetics box model using the Master Chemical Mechanism constrained by measured species and compare our results to those measured. Our results demonstrate the importance of deposition processes, including HORONO₂ uptake and loss to the aerosol phase. The results indicate that without aerosol mass, the model overpredicts daytime IN and MTN by close to a factor of two, especially in the early afternoon when aerosol number concentrations are highest. Including depositional loss of IN and MTN to the available aerosol mass as a function of time results in better agreement between the modeled and measured concentrations. These results emphasize the importance of RONO₂ multiphase chemistry and likely hydrolysis of HORONO₂ in biogenic SOA particles in controlling the NO_x and thus ozone budgets in forested environments.

9AC.18

An Isomer-Resolved Picture of Evolving Organic Aerosol Composition during Heterogeneous OH-Oxidation under Different OH concentrations and Timescales. ZIXU ZHAO, Haofei Zhang, *University of California, Riverside*

Heterogeneous hydroxyl radical (OH) oxidation of organic aerosols (OA) and the subsequent reaction pathways are a critical but poorly understood question for predicting OA's climate and air quality impacts. The complexity of the oxidation products from various pathways along multiple generations has largely hindered a coherent understanding. These products are usually multifunctional and contain structural isomers, adding analytical challenges for unambiguous separation and identification. Further, elucidating the difference of OA composition under different gas-phase OH concentrations, relative humidities (RH), and reaction timescales could be highly relevant to the real atmosphere. In order to address these questions, heterogeneous OH-oxidation of OA model compounds (glutaric acid and adipic acid) were studied in flow tube reactor (FTR) and continuous-flow stirred tank reactor (CFSTR) under identical conditions, except that the residence time differs by a factor of 60. Two RH conditions are studied (30% and 80%). In these experiments, the reaction kinetics was determined by an online thermal desorption time-of-flight chemical ionization mass spectrometer (TD-TOF-CIMS); the isomer-resolved composition of oxidation products was measured by an offline electrospray ionization ion mobility spectrometry mass spectrometer (ESI-IMS-TOFMS). From our measurements, highly dynamic product formation distributions were observed, varied with OH concentration, RH, and reaction timescales. The dramatic difference was evident in both the molecular dimension (m/Q) and the isomeric dimension. Mechanisms are proposed to explain the dynamic OA evolution. The outcome of this work will expand the currently limited mechanistic understanding of OH-initiated OA heterogeneous oxidation into a broader context.

9AC.19

Toward Development of a Metric to Relate Molecular Characteristics with Optical Properties for Biomass Burning Aerosol. NISHIT SHETTY, Apoorva Pandey, Simeon Schum, Maryam Khaksari, Lynn Mazzoleni, Rajan K. Chakrabarty, *Washington University in St. Louis*

Emissions from biomass burning are a significant source of light-absorbing organic aerosol, also called brown carbon (BrC), in the atmosphere. The complex composition of these aerosols along with source dependent diversity of BrC impedes quantitative predictions of the contribution of BrC light absorption to overall atmospheric radiative forcing. In addition to this, most models have computational limitations while incorporating a large amount of chemical detail in simulations underscoring the need for concise metrics which can capture the complexity of such aerosols to a good degree. Past studies have tried to capture the vast chemical information of organic aerosols using concise metrics such as the overall carbon oxidation state as a representation of the oxidative age of the aerosol. However, no attempts have been made to develop a concise metric to relate chemical composition to the optical properties of organic aerosols.

Here, we generated BrC aerosol from smoldering combustion of peat, cattle dung, and acacia wood. Optical properties of the emitted aerosol were characterized using multi-wavelength photoacoustic spectroscopy and ultraviolet-visible (UV-Vis) spectrophotometry on particle-laden filter samples. Molecular characterization of the aerosol extracts was performed using ultrahigh resolution mass spectrometry with both atmospheric pressure photoionization (APPI) and electrospray ionization (ESI). APPI provided chemical information for the nonpolar compounds which are otherwise not observed in the commonly-used ESI ionization technique. We explored several different chemical metrics such as the average oxidation state and mean molecular mass and compared their evolution with varying optical parameters such as the Absorption Ångström Exponent and complex refractive index of aerosols. We will present our findings on the correlation of these parameters.

9AC.20

Formation of Reactive Oxygen Species by Size-Segregated Particles Collected in Forest and Urban Environments. BRIAN HWANG, Ting Fang, Michihiro Mochida, Manabu Shiraiwa, *University of California, Irvine*

Reactive oxygen species (ROS) including hydroxyl (OH), superoxide (O₂), and organic radicals play a central role in chemical aging of ambient organic aerosols and mediating physiological processes. Environmentally persistent free radicals (EPFRs) are stable radicals with similar chemical characteristics as semiquinones and are important ROS sources in water. Recent findings have shown that biogenic secondary organic aerosols release OH and organic radicals by decomposition of organic hydroperoxides and Fenton-like reactions of metal ions with organic hydroperoxides. The sources of ROS and how various chemical components in ambient particles with different particle sizes from biogenic and anthropogenic sources influence ROS formation are not well understood. In this study, ambient size-segregated particles were collected in a forest site in Japan, where biogenic SOA are major component of ambient particles. EPFRs are directly measured from the particles on filters using an electron paramagnetic resonance (EPR) spectrometer. A spin trapping technique is applied to measure OH·, O₂·, and organic radicals from aqueous filter extracts using EPR. In addition, we plan to collect size-segregated particles in the Los Angeles basin and conduct same EPR analysis. We investigate how different chemical nature in forest and urban sites affect ROS formation by ambient particles with different particle sizes.

9AC.21

Secondary Aerosol Formation from Oxidation of Dimethyl Selenide. ROYA BAHREINI, Alexander Frie, Ying-Hsuan Lin, C.M. Sabbir Ahmed, *University of California, Riverside*

Methylation of selenium by microorganisms in soils, wetlands, lakes, or oceans and through plant metabolism results in atmospheric emissions of volatile selenium, predominantly in the form of dimethyl selenide (DMSe). Although gas phase oxidation kinetics of dimethyl selenide with major oxidants are known, the atmospheric fate of its oxidation products and the potential to form aerosol particles have not been investigated before. To increase understanding of DMSe's atmospheric fate, we performed its photooxidation (in the presence of nitric oxide) and ozonolysis in an environmental chamber. DMSe-derived aerosol was formed under both conditions, but higher yields were obtained in the photooxidation experiment. Bulk composition measurements of the aerosol using a time-of-flight aerosol mass spectrometer revealed that ~50% of the secondary aerosol mass in both experiments was from selenium containing fragments in the form of SeO₂⁺, SeC_xH_y⁺, and SeC_xH_yO⁺ (where x, y, and z are integers). Aerosol density and overall composition were similar in both experiments, suggesting similar types of oxidation products were involved in aerosol growth. Atmospheric implications of these observations will be discussed.

9AC.22

Healthy and Aphid-stressed Shrubby Plant (*Baccharis salicifolia*) Metabolomics Impact on Produced Biogenic Secondary Organic Aerosol. FATEMEH KHALAJ, Celia Faiola, Kailen Mooney, Swarup China, Christopher Anderton, Alber Rivas-Ubach, *University of California, Irvine*

Plants emit ~90% of hydrocarbons into the atmosphere globally, called biogenic volatile organic compounds (BVOCs). Climate change stressors enhance and modify plant metabolism with associated effects on BVOC emissions, and consequently, secondary organic aerosol production. However, the influence of plant stress on SOA production is not well understood. This project was the first to concurrently characterize changes in the plant metabolome and SOA production from healthy and aphid-stressed riparian shrubs *Baccharis salicifolia*—a common shrub found near rivers in California, an environment particularly susceptible to a changing climate and human influence—.

SOA was generated from *Baccharis* emissions using an Aerodyne, Inc. oxidation flow reactor (OFR). Particle composition and size distribution measurements were conducted with ACSM (Aerosol Chemical Speciation Monitor) and SMPS (Scanning Mobility Particle Sizer), respectively. BVOCs at the OFR inlet were characterized via thermo-desorption gas chromatography mass spectrometry (TD-GC-MS). On average, ten and five plants were used for healthy and stressed experiments, respectively, to generate SOA mass yield curves targeting particle concentrations ~1-13 $\mu\text{g m}^{-3}$. Each healthy and stressed experiment was repeated four times with a different set of plants. At the end of each particle generation experiment, plant leaves from all plants in the enclosure were harvested separately, flash frozen in liquid nitrogen and analyzed off-line with liquid chromatography mass spectrometry at the Environmental Molecular Science Laboratory.

SOA mass yield curves were generated for the emission profile from both healthy and stressed plants, and SOA yields varied from 1-7% in both groups. Based on the leaf-level metabolome analysis via principal component analysis (PCA), there was a clear difference in the leaf-level metabolome between the aphid-stressed and control plants.

9AC.24

NO₃-initiated Oxidation of Isoprene: Oxidation Mechanism and Aerosol Formation. BELLAMY BROWNWOOD, Juliane Fry, *Reed College*

Secondary organic aerosol from NO₃-initiated isoprene oxidation in nighttime conditions has been thought to be extremely low, due to the high volatility and small size of the isoprene precursor. Previous studies have showed low but highly variable secondary organic aerosol (SOA) yields. We present alkyl nitrate and SOA yields measured in the Reed Environmental Chamber (REC) and Simulation of Atmospheric PHotochemistry In a Large Reaction Chamber (SAPHIR) under varying chemical regimes (RO₂ + RO₂, RO₂ + NO₃, RO₂ + HO₂, and RO₂ unimolecular reactions) and varying total aerosol mass loading. In the smaller REC chamber, we observe low organonitrate yields, around 10% total (gas + particle) alkyl nitrate (AN) yield. In contrast, in the larger SAPHIR Chamber we observe consistently higher organonitrate molar yields of ~40%. We model observed yields in terms of absorptive partitioning and assess partitioning coefficients (K_p). Observed differences in yields and partitioning across the two chambers may be due to proportionally much higher wall losses in the smaller chamber when aerosol loading is low.

9AC.25**Particle, Volatile Organic Compounds and Polycyclic Aromatic Hydrocarbon Emission Flaring from Hydrofracking.**

OLANREWAJU WASIU BELLO, Thi Duong Bui, Benjamin Savareear, J. James Harynuk, Larry W. Kostiuik, Jason S. Olfert, *University of Alberta*

The world is concern about the potential impacts of hydraulic fracturing which releases a large volume of wastewater or flow-back water and produced water, a contaminant that finds its way into the environment by mixing with flared gases and water bodies. The main concern of this study is the mixture of the flow-back and produced water with flares in an aerosolized form. When they mix with flares, they produce toxic materials, substances that deplete our ozone layer and greenhouse gases. Volatile organic compound (VOCs) and polycyclic aromatic hydrocarbon (PAHs) are the main substances of those aforementioned produces.

A primary emission measurement has been carried out on a lab-scale flare, where Methane (CH_4) and Propane (C_3H_8) are the two hydrocarbons used in this study. A photoacoustic extinctionsmeter (PAX) was used to measure the amount of black carbon (BC) emitted by the flare, and a NO_x analyzer was used to measure the concentrations of NO , NO_2 and NO_x present in the flare. Also, exhaust gases were collected in a Tedlar bag for gas chromatographic analysis to know the amount of CO , CO_2 and hydrocarbon present in the flared gases.

Also, preliminary qualitative and quantitative analyses of VOCs and PAHs in the gas and particulate phases were carried out using thermal desorption coupled to comprehensive two-dimensional gas chromatography with flame ionization detection and time-of-flight mass spectrometry (TD-GC \times GC-FID/TOFMS). Thermal desorption provides a less tedious way of sample collection and introduction to the GC, as well as reduces the time and cost of analyses compared to traditional liquid extraction methods. The comprehensive two-dimensional GC is superior to conventional one-dimensional GC by better peak capacity and sensitivity. Furthermore, a mass spectrometer enables a direct identification of the analytes.

9AC.26**Heterogeneous Chemistry of CaCO_3 Aerosols with HNO_3 and HCl .** HAN HUYNH, V. Faye McNeill, *Columbia University*

Calcite (CaCO_3) particles have previously been proposed for use in stratospheric solar radiation management (SRM, Keith et al. PNAS 2016). They also serve as a proxy for calcium-rich mineral dust. We investigated the heterogeneous reactions of submicron CaCO_3 particles with HNO_3 and HCl in a flow reactor. The particles were aerosolized using dry dispersion and impacted on ZnSe windows, where they were exposed to the reagent gases at stratospherically relevant concentrations, at 296 K and under dry conditions. The chemical composition of the particles was analyzed before and after trace gas exposure using Fourier transform infrared spectroscopy (FTIR). The particle size distribution was characterized prior to deposition using a scanning mobility particle sizer (SMPS) and a micro orifice uniform deposition impactor (MOUDI).

A $\text{Ca}(\text{OH})(\text{HCO}_3)$ termination layer was detected in the form of a HCO_3^- peak in the FTIR spectra, indicating adsorption of water molecules on the surface. The results demonstrate the reaction of HNO_3 with $\text{Ca}(\text{OH})(\text{HCO}_3)$ to produce $\text{Ca}(\text{NO}_3)$ and carbonic acid. HCl reacted with $\text{Ca}(\text{OH})(\text{HCO}_3)$ to produce CaCl_2 and carbonic acid. The depletion of the $\text{Ca}(\text{OH})(\text{HCO}_3)/\text{Ca}(\text{CO}_3)$ signal due to reaction with HCl or HNO_3 followed pseudo-first order kinetics. Reactive uptake coefficients will be presented and implications for stratospheric ozone in a SRM scenario will be discussed.

9AC.27

ISORROPIA-MCX: Implementation of the Multicomplex Variable Method into the Aerosol Thermodynamic Model, ISORROPIA. BRYAN BERMAN, Isaiah Sauvageau, Shannon Capps, Ryan Russell, *Drexel University*

Sensitivity analysis using atmospheric chemical transport models provides a deeper understanding of how specific emissions affect pollutant concentrations. Given a model with emissions as inputs and pollutant concentrations as outputs, this analysis is achieved by computing the partial derivatives of the underlying functions with respect to their input variables. Implementing higher-order sensitivity calculations can be quite difficult even though they are important to understanding nonlinear processes. A novel approach to sensitivity analysis leverages multicomplex variables to improve accuracy over the finite difference method and ease of implementation over the decoupled direct method (DDM).

Here, the multicomplex variable method (MCX) is implemented in the inorganic aerosol thermodynamic equilibrium model, ISORROPIA, which treats the Na^+ - SO_4^{2-} - HSO_4^- - NH_4^+ - NO_3^- - Cl^- - H_2O aerosol system (ISORROPIA-MCX). Specifically, the first- and second-order sensitivities of an inorganic species in the aerosol or gaseous phase with respect to the total concentrations are calculated. ISORROPIA-MCX is beneficial because there are enough inputs and outputs to demonstrate a main advantage of the method, which is simultaneously calculating multiple sensitivities. This is useful for understanding many atmospheric processes such as determining how much an aerosol constituent influences aerosol acidity. Furthermore, the ability to compute higher order derivatives is useful when the functions are nonlinear as it avoids subtractive cancellation and numerical round-off errors. Since thermodynamics is a nonlinear process and ISORROPIA uses nonlinear functions, we demonstrate the advantages of calculating higher order sensitivities using MCX. This work demonstrates the multi-complex variable method in ISORROPIA and shows its utility for investigating aerosol acidity

9AC.28

Degradant Formation in Cannabis Concentrate Aerosols. ALISHA ORTIZ, Jiries Meehan-Atrash, Robert Strongin, *Portland State University*

Vaporizing cannabis extracts has increased in popularity as a potentially healthier alternative to smoking. Despite the rise in consumption by this method, little is known about the chemical profiles of aerosolized extracts. Our lab has worked on identifying degradation products and mechanisms or formation therein as a function of naturally-occurring components or additives. Given the unique chemical makeup of cannabis-derived aerosols as compared to those derived from cigarettes or e-cigarettes, our focus has been on collection techniques and gas-particle partitioning of the products found.

9AC.29

Growth and Evaporation Kinetics of Secondary Organic Aerosol as a Function of Relative Humidity. RAHUL ZAVERI, John Shilling, Alla Zelenyuk, Maria Zawadowicz, Kaitlyn J. Suski, Swarup China, Daniel Veghte, Alexander Laskin, *Pacific Northwest National Laboratory*

Low bulk diffusivity inside viscous semisolid atmospheric secondary organic aerosol (SOA) can prolong equilibration timescale as well as influence aerosol growth kinetics and the associated size distribution evolution. We present here quantitative insights into the effects of bulk diffusivity on the growth and evaporation kinetics of isoprene SOA as a function of relative humidity (RH). A series of chamber experiments of SOA formation from photooxidation of isoprene were carried out in the presence of bimodal aerosol seeds consisting of Aitken mode composed of potassium sulfate and accumulation mode composed of aged α -pinene SOA. Evaporation kinetics indicate that isoprene SOA is composed of several semivolatile organic compounds (SVOCs). Model analysis shows that while liquid-like bulk diffusivities can be used to fit the observed evaporation kinetics, they fail to explain the growth kinetics of bimodal aerosol by significantly under-predicting the evolution of the Aitken mode. In contrast, lower bulk diffusivity values corresponding to viscous semisolids can successfully reproduce 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. The estimated effective bulk diffusivity was found to experience only a 4-fold increase as the RH increased from 0 to 75%, suggesting that aged α -pinene SOA was quite viscous even at 75% RH—contrary to published literature. These results have important implications for modeling SOA formation and growth of ultrafine particles under ambient conditions.

9AC.30

Chemical Role of Water on Secondary Organic Aerosol Formation and Ageing. CHRISTOPHER SNYDER, Giuseppe Petrucci, *University of Vermont*

Secondary organic aerosols (SOA) make up a significant fraction of the aerosol mass burden, yet our fundamental understanding of their roles in atmospheric processes remains limited. Recent laboratory studies suggest that the physical and chemical properties of some SOA may be driven by the presence of water at different stages of the SOA lifecycle (i.e. particle genesis vs. chemical aging). However, recent evidence suggests that bulk chemical metrics, such as O:C ratio, are not always sufficient to accurately predict these SOA properties and that a molecular level understanding is needed to better understand the mechanisms, chemical and physical, by which atmospheric SOA impacts Earth's atmosphere. We present initial results on the characterization of a dual-chamber system designed to separate particle genesis from aging, permitting each process to be studied independently. Furthermore, soft ionization aerosol mass spectrometry was used to measure chemical composition of SOA under varying conditions of relative humidity during and post particle formation. Herein we describe challenges with the reproducible generation of SOA, as well as the unexpectedly dominant role of mixing within the chamber in impacting particle physical and chemical properties. Finally, as proof-of-principal of this innovative design, results are presented for compositional differences in SOA, as well as SOA yields and particle size distributions, generated from ozonolysis of the green leaf volatiles *cis*-3-hexenyl acetate (CHA) and *cis*-3-hexenol (HXL). Preliminary results show SOA yield decreases as humidity increases. For HXL, SOA yield dropped from 5.4% at low humidity to 2.4% at high humidity. The difference in SOA yield was more drastic for CHA going from 2.2% at low humidity to 0.2% at high humidity.

9AC.32

Using GECKO-A to Study Secondary Organic Aerosol Formation from Camphene Relative to α -Pinene and Limonene. ISAAC AFREH, Bernard Aumont, Marie Camredon, Kelley Barsanti, *University of California, Riverside*

Camphene has been measured in emissions from a variety of biogenic sources, including vegetation, marine samples, and soils. Additionally, camphene has been identified as a dominant monoterpene in biomass burning emissions from different fuel types during laboratory and field studies. Despite the contribution of camphene to ambient emissions, very little is known about the potential of camphene to form secondary organic aerosol (SOA). Relative to other monoterpenes, α -pinene and limonene for example, camphene has been significantly understudied in smog chambers. The lack of chamber-derived SOA data for camphene may lead to significant uncertainties in predictions of SOA from monoterpenes using existing parameterizations in air quality models, given the reported contributions of camphene to biogenic and smoke emissions. In this work, GECKO-A, an explicit chemical mechanism generator and SOA box model, was used to study SOA formation from camphene. Model predictions for camphene were compared with predictions for α -pinene and limonene, since more data exist for measurement-model comparison. GECKO-A simulations were performed under chamber-relevant and atmospherically-relevant conditions to enable comparison between the monoterpenes, as well as comparison with published data. Results to be presented include: i) simulated SOA mass and yield for each monoterpene; ii) gas- and particle-phase volatility distributions; and iii) mass contribution of product species to total SOA as a function of carbon number. Also, comparisons between simulated SOA yields and published SOA yields under relevant chamber conditions will be presented. GECKO-A based SOA studies of camphene will help improve representation of monoterpene chemistry in air quality models, thereby leading to more accurate predictions of the contributions of monoterpene-derived SOA to fine particulate matter (PM_{2.5}).

9AC.33

Simulation of SOA Formation Using Gas-Wall Process Free Model parameters in the Presence of Inorganic Salts Containing Electrolytes under Various NO_x Levels. SANGHEE HAN, Myoseon Jang, *University of Florida*

The Gas-Wall Process (GWP) is known to have a large impact on the prediction of Secondary Organic Aerosol (SOA) yields due to the bias of the semiempirical model parameters obtained from the chamber studies. Recently, our research team launched the GWP model using the Quantitative Structure Activity Relationship (QSAR) to predict the impact of chemical structure on GWP under the various humidity conditions. Our laboratory's research efforts have also improved the state-of-the-science-art via the development of the UNified Partitioning-Aerosol phase Reaction model (UNIPAR), which features partitioning in multiphase and emerging chemistry in the aerosol phase. However, the model parameter in the preexisting UNIPAR inherits the impact of GWP due to the GWP biased chamber data. In this study, the GWP model integrated with QSAR is applied to the UNIPAR model to improve the model parameters. The resulting model parameters are applied to various SOA systems that are produced via the photooxidation of different hydrocarbons under varying NO_x, inorganic seed aerosol, and humidity conditions. The impact of GWP on SOA formation is also evaluated by comparing the predicted SOA mass using the model parameters without GWP and that using the model parameters inheriting GWP. The characteristic time analysis of various processes including partitioning, gas-phase reactions, and aerosol phase reactions suggests that the impact of GWP on SOA formation is relatively small in the presence of the inorganic seeds compared to that without aqueous reactions.

9AC.34

Effects of Emission Reduction on Air Pollution in India. HAO GUO, Sri Kota, Hongliang Zhang, *Louisiana State University*

With the rapid growth of industries and population in India, increase of air pollutants emissions is expected and will result in higher pollution levels in future than nowadays without proper control measurements. This study will investigate the effects of emission reduction on concentrations of ozone and particulate matter (PM) in India, 2015 using the Community Multi-scale Air Quality (CMAQ) model. The meteorology will be generated using Weather Research and Forecasting (WRF) model version 3.7.1 and 9 emission scenarios will be developed based on Emissions Database for Global Atmospheric Research (EDGAR) version 4.3 as following: 10%, 20%, 30% to 90% reduction of national wide anthropological emissions. The differences in spatial variations of air pollutants between reduction and non-reduction scenarios will be analyzed. The results will be helpful to develop emission control measurements to reduce air pollution in India.

9AC.35

Isoprene Effects on Biogenic and Inorganic New Particle Formation. LEE TISZENKEL, Ryan Haley, Shanhu Lee, *University of Alabama Huntsville*

New particle formation (NPF) via gas-to-particle conversion is a ubiquitous event that is responsible for about 50% of the global CCN production. Oxidized organic species such as alpha-pinene and inorganic species such as sulfuric acid and ammonia have been observed to participate in NPF in areas with a sufficient concentration of these precursors. However, the presence of high concentrations of isoprene, which is the most abundant biogenic volatile organic compound (BVOC) globally, may suppress the NPF process, although the chemical mechanisms behind this suppression processes are not yet known. Here we present the results of laboratory studies of both organic and inorganic nucleation in the presence of varying ozone levels, isoprene and pure hydrogen gas acting as a hydroxyl radical scavenger, using a fast flow nucleation reactor. These experiments are conducted with a flow tube nucleation reactor monitored by a particle size magnifier (PSM) that produces size distributions between 1 and 3 nm, a scanning mobility particle sizer (SMPS) that produces size distributions from 3 to 100 nm, and chemical ionization mass spectrometers (CIMS) that monitor sulfuric acid and amine/ammonia concentrations. Varying ozone during these experiments allows for varying concentrations of highly oxidized molecules (HOMs) that participate in biogenic NPF and HOMs concentrations are calculated using the steady state condition in the flow tube. Isoprene effects on nucleation in the presence of both organic and inorganic precursors at atmospherically relevant concentrations will be discussed.

9AC.37

Investigations of the Mixing of Sulfate Aerosols and Isoprene Epoxydiols in Secondary Organic Aerosol Formation Chamber Experiments. THEODORA NAH, Lu Xu, Kymberlee Osborne-Benthaus, S. Meghan White, Stefan France, Nga Lee Ng, *City University of Hong Kong*

The impacts of inorganic sulfate aerosol mass and mixing conditions on SOA formed from the reactive uptake of trans- β -IEPOX under humid conditions were investigated in this laboratory chamber study. For both highly acidic and less acidic seed aerosols, SOA mass concentrations increased with sulfate mass. Higher SOA mass concentrations were measured in experiments where highly acidic seed aerosols were used. In addition, the SOA mass concentration and composition depended on how IEPOX and sulfate seed aerosols were mixed in the chamber, which was investigated by varying the injection order of sulfate seed aerosols and IEPOX (i.e., injection of IEPOX first vs. injection of seed aerosols first). Higher SOA mass concentrations were measured in experiments where sulfate seed aerosols were introduced into the chamber before IEPOX. This indicated that SOA formed in "seed aerosols first" experiments contained larger quantities of low volatility organic compounds compared to SOA formed in the "IEPOX first" experiments. Overall, these results indicated that IEPOX-derived SOA formed in chamber experiments will depend on the amount of sulfate seed aerosols used and mixing conditions in the chamber.

9AC.38

Photolysis of Aqueous Atmospheric Aerosol Mimics. MELISSA GALLOWAY, Jacqueline Sharp, Shiqing Ma, Joseph Woo, *Lafayette College*

Aqueous reactions of small, water soluble aldehydes with amines or ammonium salts have been shown to be important for atmospheric brown carbon formation processes. The extent to which photolysis of these brown carbon compounds changes the chemical composition and light absorption of these systems is not well understood or characterized. We photolyze aged reaction systems of aqueous carbonyls (e.g., glycolaldehyde, glyoxal, methylglyoxal, and hydroxyacetone) and ammonium sulfate and monitor light absorption and chemical composition via UV-visible spectroscopy and mass spectrometry. Photobleaching and photobrowning rates vary with wavelength and aldehyde identity, while mass spectrometry shows that the chemical composition changes significantly upon photolysis.

9AC.39

Effects of Relative Humidity and Aerosol Liquid Water on the Molecular Composition and Aging of Secondary Organic Aerosols. CYNTHIA WONG, Lauren Fleming, Julia Montoya-Aguilera, Sergey Nizkorodov, *University of California, Irvine*

Relative humidity (RH) and aerosol liquid water may have competing effects on secondary organic aerosol (SOA) formation. Elevated RH can alter the mechanism of gas-phase oxidation of volatile organic compounds, in which SOA are formed, and suppress oligomer formation in particles. Aerosol liquid water, on the other hand, can help oxidize the water soluble gases that partition into the aqueous phase, thereby increasing the particle mass concentration. After the particles are already formed, presence of water can alter the mechanisms of spontaneous and photochemical aging processes in particles. The goal of this work is to systematically explore the effects of water vapor and aerosol liquid water on the chemical composition of SOA during formation and aging. SOA from α -pinene ozonolysis were generated in a flow tube reactor in four different ways: in the presence and absence of ammonium sulfate seeds, and at <2% and 90% RH. Samples were either aged in dry or humid conditions for several days or analyzed immediately with direct analysis in real-time (DART) and electrospray ionization (ESI) mass spectrometry, to provide information about the chemical composition of SOA before and after aging. The patterns of peak intensities and observed molecular formulas were examined for evidence of water-driven chemistry. The results from this study should help decouple the effect of gaseous and liquid water on the chemical composition and properties of SOA, and ultimately improve our understanding of SOA formation and aging processes.

9AC.40

Role of Particle Composition in the Heterogeneous Reactivity of Carboxylic Acid Aerosol. REBECCA RAPF, Kevin Wilson, *Lawrence Berkeley National Laboratory*

The oxidation of organic aerosols in the atmosphere is depends strongly on heterogeneous reactions that are governed by the composition of the aerosol. The reactive fate of carboxylic acid molecules in aerosol is controlled both by exposure to gas-phase oxidants, but also by the nature of the particle phase. For instance, previous modeling studies suggest that acid-base chemistry of an aqueous particle may be competitive with oxidation under some conditions, and this branching between chemical pathways may manifest in the physical characteristics of the particle itself, such as its size. Similarly, changes in molecular packing at the interface can change the heterogeneous reactivity of a particle. Packing and orientation of molecules at the surface is highly dependent on molecular properties, such as the cis- or trans- isomerization of unsaturated carboxylic acids. Direct Analysis in Real Time (DART) ionization mass spectrometry is coupled to a flow tube reactor to monitor the heterogeneous oxidation of size-selected organic aerosols. We report here on the effect of environmental conditions, such as pH, on the heterogeneous oxidation of model systems, including citric acid, and the competition with other pathways, such as acid-base chemistry. Additionally, through analysis of particle size following interaction with the DART source, a probing depth can be calculated, allowing for monitoring surface-sensitive reactions.

9AC.41

An Integrated Organic Aerosol Simulation: From Volatile Precursors to Cloud Droplet Formation. KYLE GORKOWSKI, Camilo Damha, Dalrin Ampritta Amaladhasan, Thomas Preston, Andreas Zuend, *McGill University*

The water uptake characteristics of an atmospheric organic aerosol particle are among the properties controlled by chemical composition. The aerosol chemical composition is dependent on the atmospheric chemical processing of emitted volatile organic compounds (VOCs) and primary organic aerosol. To probe the links between emitted VOCs, the resulting organic aerosol species, and water uptake, we built an integrated organic aerosol simulation.

The activity coefficient model used is the Binary Activity Thermodynamics model (BAT), which is a water-sensitive, reduced-complexity organic aerosol thermodynamics model. A Volatility Basis Set framework (VBS) is combined with the BAT model, allowing predictions of RH-dependent organic co-condensation, liquid-liquid phase separation, and cloud droplet activation. Our VBS+BAT model is then run on outputs from the Master Chemical Mechanism (MCM), which is a near-explicit chemical mechanism describing key gas-phase chemical processes of VOCs. The simulation starts at primary VOC chemical reactions and ends at cloud droplet formation characteristics.

Using this setup, we will present simulations with different initial VOC concentrations of isoprene, alpha-pinene, and toluene. We will discuss how variations in precursor concentrations are linked to changes in water uptake and cloud droplet activation behavior. The simulated hygroscopicity parameters will be compared to measured hygroscopicity parameters for each system. In addition to the VOC simulations, we found good agreement between measured hygroscopicity parameters of pure component systems and the BAT model predictions.

9AC.42

Volatility Change during Droplet Evaporation of Pyruvic Acid. SARAH SUDA PETTERS, Thomas Hilditch, Sophie Tomaz, Rachael E.H. Miles, Jonathan P. Reid, Barbara Turpin, *University of North Carolina at Chapel Hill*

Atmospheric water-soluble organic gases such as pyruvic acid are produced in large quantities by photochemical processing of biogenic hydrocarbons and undergo water-mediated reactions in aerosols and hydrometeors. These reactions can contribute to aerosol mass by forming less volatile compounds. However, the additional aerosol mass contributed by aqueous reactions is highly uncertain because models use simplified partitioning mechanisms based on fixed yields or limited laboratory experiments for these systems. Here we experimentally determine the evolution of volatility distributions of pyruvic acid using both the Vibrating Orifice Aerosol Generator (VOAG) and an electrodynamic balance (EDB). Pyruvic acid was evaporated with and without oxidation by OH radicals. The evaporation behavior of oxidized mixtures was consistent with expectations based on known volatilities of reaction products. However, more surprisingly, independent VOAG and EDB evaporation experiments conducted *without oxidation* also resulted in stable residual particles; the estimated volume yield was 10–30% of the initial pyruvic acid. Yields varied with temperature and pyruvic acid concentration under cloud, fog, and aerosol-relevant conditions. The formation of low volatility products, likely cyclic dimers, suggests that pyruvic acid accretion reactions occurring during droplet evaporation could contribute to aerosol mass in the atmosphere.

9AC.43

A Scalable, Portable, Gas-Aerosol Chemistry Treatment for Atmospheric Models. MATTHEW DAWSON, Christian Guzman, Matthew West, Nicole Riemer, Mario Acosta, Oriol Jorba, Donald Dabdub, *Barcelona Supercomputing Center*

Decades of progress in the identification of increasingly complex atmospherically relevant mixed-phase physiochemical processes have resulted in an advanced understanding of the evolution of atmospheric systems, but have also introduced a level of complexity that few large-scale atmospheric models were originally designed to handle. Most regional and global models thus comprise a collection of physiochemical modules for the treatment of gas- and aerosol-phase chemistry and physics that have often been developed independently and with a focus on computational efficiency that leads to significant development efforts when modules are coupled for the first time, or new science is introduced. In addition, these modules are often tightly tied to the aerosol micro-physics scheme used by the host model, making the porting of chemical mechanisms to new models challenging.

A flexible treatment for gas- and aerosol-phase chemical processes has been developed for incorporation in models of diverse scale, from box models up to global models. A key feature of this novel framework is an abstracted aerosol representation that allows the same chemical mechanism to be solved on models with different aerosol representations (e.g., binned, modal, or particle-resolved). This is accomplished by treating aerosols as a collection of condensed phases that can be implemented according to the aerosol representation of the host model. The framework also allows multiple chemical processes (e.g., gas- and aerosol-phase chemical reactions, emissions, deposition, photolysis, and mass-transfer) to be solved simultaneously as a single system. In 3-D models, multiple grid cells can also be treated as a single chemical system and solved simultaneously, thus improving model performance. The flexibility of the model is achieved through a combination of JSON input files and run-time model configuration. JSON format is widely used for structured data, and allows entire gas- and aerosol-phase chemical mechanisms to be described in human-readable format, with as much complexity as is required to describe the system. Run-time model configuration allows changes to be made to any part of the chemical mechanism without recompiling the model. This new treatment has been developed using the PartMC modeling framework and deployed in the NMMB-MONARCHv2.0 chemical weather prediction system for use at global and regional scales. Results from the initial deployment to NMMB-MONARCHv2.0 will be discussed, along with extension to more complex gas-aerosol systems, and the use of GPU-based solvers.

9AC.44

H₂SO₄-H₂O Binary and H₂SO₄-H₂O-NH₃ Ternary Homogeneous and Ion-mediated Nucleation: Lookup Tables and Comparisons with CLOUD Measurements. FANGQUN YU, Alexey Nadykto, Gan Luo, Jason Herb, *The State University of New York at Albany*

New particle formation is a key source of atmospheric particles which have important implications for air quality and climate. Recently, we have developed a comprehensive kinetically-based H₂SO₄-H₂O-NH₃-Ions nucleation model that is based on the thermodynamic data derived from both quantum-chemical calculations and laboratory measurements. The model captures well the absolute values of nucleation rates as well as the dependence of nucleation rates on concentrations of NH₃ and H₂SO₄, ionization rates, temperature, and relative humidity observed in the well-controlled Cosmics Leaving Outdoor Droplets (CLOUD) measurements. Here we employ this recently developed kinetic nucleation model to generate nucleation rate look-up tables for H₂SO₄-H₂O binary homogenous nucleation (BHN), H₂SO₄-H₂O-NH₃ ternary homogeneous nucleation (THN), H₂SO₄-H₂O-Ions binary ion-mediated nucleation (BIMN), and H₂SO₄-H₂O-NH₃-Ions ternary ion-mediated nucleation (TIMN). The look-up tables cover a wide range of key parameters that can be found in the atmosphere, and their usage significantly reduces the computational costs of the BHN, THN, BIMN, and TIMN rate calculations, which is critical for multi-dimensional modeling. The look-up tables can also be used by those involved in experiments and field measurements to quickly assess the likeliness of inorganic nucleation involving H₂SO₄, H₂O, NH₃, and Ions. The lookup tables have been incorporated into three widely used community CESM-CAM5, GEOS-Chem, and WF-Chem and examples of nucleation rates are presented.

9AC.45

Day and Night Variability of Carbonaceous Aerosols over Urban Region of Northern India. ATAR SINGH PIPAL, Ajay Taneja, Dr. B. R. Aambedkar University, Agra, India

The organic carbon (OC) and elemental carbon (EC) associated with PM_{2.5} (fine particles) were investigated at a roadside, Agra, India during winter period. PM_{2.5} samples were collected for different time period i.e., 24-h, day and night by medium volume air sampler and analyzed for OC and EC using thermal optical transmittance protocol (Sunset- Lab). Average mass concentration of PM_{2.5} was $183 \pm 114 \mu\text{g m}^{-3}$, varied from 29 to $612 \mu\text{g m}^{-3}$. Carbonaceous analysis results showed that the average concentration of OC varied from 39 to $96 \mu\text{g m}^{-3}$ for 24-h, 71 to $89 \mu\text{g m}^{-3}$ for day and 64 to $91 \mu\text{g m}^{-3}$ for night while EC varied from 3.4-9.3 $\mu\text{g m}^{-3}$, 8.9-16.8 $\mu\text{g m}^{-3}$ and 12.4-18.2 $\mu\text{g m}^{-3}$ for 24-h, day and night respectively. Estimated OC/EC was varied between 4.9 and 47 which suggest the presence of secondary organic aerosol (SOA) over the receptor area. Both OC and EC accounts for 43% of the total PM_{2.5} mass in which OC contributed major part (38 %) while EC contributed 5 % only. In order to know day and night variation relative abundance of OC and EC was higher during day time due to vehicular emissions. Beside this high biomass burning, fossil fuel combustion could not be ignored as study was conducted during winter period. During winter people burn bio-fuels for cooking and also used to protect from the cold. Significant correlation among OC (0.83) and EC (0.97) to PM_{2.5} was observed for 24-h samples, indicates the similar sources. Being high loading of OC and EC associated with fine particles inferred very unsafe air quality for human health as well as regional climate change. It is also suggested to take necessary and immediate action in mitigation of the emission of carbonaceous aerosol in the northern part of India.

9AP.1

The Light Scattering Study of Highly Absorptive Hematite Aggregates. PRAKASH GAUTAM, Justin Maughan, Christopher Sorensen, Kansas State University

We present a measurement of the light scattering of highly absorptive hematite particles, which have agglomerated irregular shapes. The measurements were made at a wavelength of 532 nm in the scattering angle range from 0.3° to 158°. Hematite is important from a light scattering point of view because it has high values of the real and imaginary parts of the refractive index $m = n + ik = 3 + i0.5$ at the studied wavelength. Scanning electron micrographs are used to determine size distribution. The mean aggregate size is 4-5 micron, roughly a diameter, and the aggregate is composed of smaller grains with approximate size of 200 nm. Mie calculations for a sphere equivalent to the aggregate size of hematite particles were compared to the experimentally observed results. The observed results showed an enhanced backscattering, whereas the Mie calculations did not due to the large imaginary part of the refractive index. We simulated the agglomerate hematite particles by assuming it was composed of spherical monomers inside a spherical volume. Then the light scattering was calculated using the T-matrix method. The calculated results showed an enhanced backscattering. This suggests that an enhancement in the backscattering is due to the effect of multiple scattering between the grains within the aggregates.

9AP.2**The Effect of Particle Size on Aerosol Concentration.**

TERRENCE GARCIA, Ashley Alli, Sabrina MAJ McGraw, *Laulima Government Solutions*

Particle size is one of the key components for characterizing the behavior of aerosols, particularly in regards to the dose received by an animal. Different sizes of aerosolized particles result in a difference in aerosol concentration, which is effected by the mass concentration and the number concentration. All of these factors can have an effect on the dose due to the quantity and quality of particles that the subject may inhale. The size, number and mass of the aerosolized particles will all have an impact on particle deposition. Aerosolized particles deposit in the respiratory system by impaction, sedimentation and diffusion. The predominant method of deposition is influenced by the particle size. Larger particle sizes deposit in the nasopharynx or upper respiratory tract. In contrast, smaller particles deposit in the lower respiratory tract. However, a particle size that is too small will result in no or limited deposition. Due to the significant influence particle size has on deposition, we evaluated a wide range of particle sizes to determine aerosol concentration as it relates to of mass and number concentration.

9AP.3**The Dependence of the Optical Properties of Soot Aggregates on Their Morphological Mixing State.**

OGOCHUKWU ENEKWIZU, Divjyot Singh, Mary McGuinness, Alexei Khalizov, *New Jersey Institute of Technology*

Soot nanoparticles, produced from the incomplete combustion of fossil fuels, absorb solar radiation and contribute to climate change by direct radiative forcing. The magnitude of forcing is strongly influenced by the changes in morphology and mixing state of the soot aggregates as they interact with other aerosols during atmospheric transport. However, previous studies on soot optical properties have been largely inconclusive because a systematic examination of the sensitivity of the optical properties of soot to aerosol mixing state has not been performed. For thinly coated soot aggregates, our previous research has shown the existence of two coating distributions (uniform condensation and capillary condensation) governed by the degree of vapor supersaturation of the condensing material. In this study, we investigate the effects of these two distinct mixing states on the light absorption and scattering of coated soot aggregates. We conduct our optical measurements at a wavelength of 530 nm on size-classified soot with different mixing states and morphologies engineered through controlled vapor supersaturation and aging experiments. We compare our results to optical calculations via Discrete Dipole Approximation (DDA) using the morphology and mixing state data derived from our experiments to numerically simulate soot aggregates and apply coating material using an algorithm that describes the aggregate in terms of dipole points. We also contrast our findings against traditionally used RDG and core-shell Mie methods for optical calculations. The outcome of our findings may help address discrepancies in previous studies and improve simulations of the radiative forcing of soot.

Keywords: soot, morphology, mixing state, light absorption, discrete dipole approximation

9AP.4

Integration of the MOSAIC Aerosol Model into the Environment and Climate Change Canada AQ Model. KIRILL SEMENIUK, Ashu Dastoor, *Environment and Climate Change Canada*

We present preliminary results from the integration of the MOSAIC aerosol model into the Environment and Climate Change Canada online air quality model, GEM-MACH. MOSAIC includes nucleation, coagulation, non-equilibrium mass transfer and thermodynamics. Three simulations with constrained meteorology are conducted with the MOSAIC version including bin-resolved, mode-aggregated (nucleation-Aitken, accumulation and coarse) and bulk treatment of the thermodynamics and inter-compared with each other and against the reference GEM-MACH model with bulk thermodynamics.

9AP.6

Individually Identifiable Aerosol Particles Using Luminescent Nanocrystals. Michael H. Stewart, Kimihiro Susumu, Jozsef Czege, Cathy S. Scotto, Alan Huston, JAY D. EVERSOLE, *Naval Research Laboratory*

Commercial polymer beads with narrow size distributions available in a wide range of mean diameters from 10's of nm to 10's of μm have become de facto particle standards with pervasive use throughout the aerosol research community. Moreover, a wide range of organic molecule dyes can also be selected to impart tailored emission profiles to these beads. This combination of diameter and excitation/emission profile selection provides capabilities for many aerosol applications, such as tracking in complex gas flows using either fluorescent imaging or fluorescent particle counting. However, for environmental applications, ambiguity remains at the individual particle level regarding whether any given particle belongs to ambient aerosol background, or a released tracer aerosol.

Here, we describe initial work to produce and characterize particles that use luminescent nanocrystals (NC's) instead of organic dyes for imparting photo-emissive properties to micron-sized particles. NC's offer significant advantages over dye molecules including: (a) narrower emission profiles (no long tails to the red), and (b) chemical and photo stability, since nanocrystals do not photo-bleach (unlike dyes). Consequently, embedding multiple separate populations of NC's, each with a distinct, non-overlapping emission profile, into a micron-sized bead sample will create a complex spectral superposition "bar-code" that can serve as an identifying optical mark on each individual bead in that sample. Such complex emission profiles cannot be emulated in natural processes. While traditional NC's (quantum dots) have previously demonstrated emission "bar code" identification for larger beads ($>20 \mu\text{m}$) [1], so far, this has not been achieved in beads small enough for aerosol use. Traditional quantum dots may also present an issue as hazardous materials for environmental releases. Our effort focuses on more recent, and more benign, NC materials, as well as new upconverting NC's [2] which can provide an additional dimension for creating unique identification signatures.

[1] For example: Yuanjin Zhao, et.al., *J. Am. Chem. Soc.*, 2011, 133 (23), pp 8790–8793, DOI: 10.1021/ja200729w.

[2] Noah J. J. Johnson, et. al., *J. Am. Chem. Soc.* 2017, 139, 8, 3275-3282 DOI: 10.1021/jacs.7b00223.

9AP.7

Modeling of Multispecies Aerosol Formation and Evolution in a Capillary Aerosol Generator. Francesco Lucci, Edo Frederix, ARKADIUSZ KUCZAJ, *Philip Morris International R&D*

The capillary aerosol generator (CAG) concept was developed nearly 20 years ago, finding various applications, including generation of pharmaceutical aerosols. In the CAG, aerosol is generated around the capillary outlet by vigorous, often turbulent, mixing of a jet of supersaturated vapors with an ambient cold air stream. Computational modeling of such a complex process remains a challenge. We have developed a computational fluid dynamics code, AeroSolved (<http://www.aerosolved.com>) for simulations of the formation, transport, evolution, and deposition of multispecies aerosol mixtures. In this work, we concentrate on development of a consistent modeling approach between aerosol nucleation and condensation/evaporation processes in a multispecies context. Assuming a dilute aerosol mixture with limited impact on the total momentum and energy, we solve the transport equations for each species and phase while treating the energy and momentum only for the total mixture as a whole. A drift flux approach is used to transport each species relative to the mixture by computing relative velocities and diffusion terms. A sectional method is used to resolve the shape of the particle size distribution without making a priori assumptions. We use modified classical nucleation theory extended for multispecies mixtures. The species-specific condensation rate function introduces a modification of the standard single-species condensation rate to account for the Stefan flow. The models are tested and validated against available literature. The validated models are finally applied to the simulation of aerosol formation in the CAG. We show that in our setup, turbulent diffusion plays an important role in the gas transport and thus in the aerosol formation. The majority of the particles is formed in a ring centred on the axis of the CAG chamber. From there, particles are transported further downstream and diffuse radially. Numerical results for varying thermodynamic conditions and parametric studies will be presented in detail.

9AP.8

Timescales of Secondary Organic Aerosols to Reach Equilibrium at Various Temperatures and Relative Humidities. YING LI, Manabu Shiraiwa, *University of California, Irvine*

Secondary organic aerosols (SOA) account for a substantial fraction of air particulate matter and SOA formation is often modeled assuming rapid establishment of gas-particle equilibrium. Here, we estimate the characteristic timescale for SOA to achieve gas-particle equilibrium under a wide range of temperatures and relative humidities using a state-of-the-art kinetic flux model. Equilibration timescales were calculated by varying particle phase state, size, mass loadings, and volatility of organic compounds in open and closed systems. Model simulations suggest that the equilibration timescale for semi-volatile compounds is on the order of seconds or minutes for most conditions in the planetary boundary layer, but it can be longer than one hour if particles adopt glassy or amorphous solid states with high glass transition temperature at low relative humidity. In the free troposphere with lower temperatures it can be longer than hours or days even at moderate or relatively high relative humidity due to kinetic limitations of bulk diffusion in highly viscous particles. The timescale of partitioning of low-volatile compounds into highly viscous particles is shorter compared to semi-volatile compounds in the closed system, as it is largely determined by condensation sink due to very slow re-evaporation with relatively quick establishment of local equilibrium between the gas phase and the near-surface bulk. The dependence of equilibration timescales on both volatility and bulk diffusivity provides critical insights into thermodynamic or kinetic treatments of SOA partitioning for accurate predictions of gas- and particle-phase concentrations of semi-volatile compounds in regional and global chemical transport models.

9AP.9

Backscattering from Fractal Aggregates. BLAINE FRY, Christopher Sorensen, Raiya Ebini, *Kansas State University*

We present studies of light backscattering from a system of aggregating fractal aggregates. Scattered light was collected between 175.5 and 184.5 degrees by a 512-channel photodiode array, as a function of time after the onset of aggregation. Results are contextualized by comparing with forward scattering and dynamic scattering to retrieve the fractal dimension and mobility radius of the aggregates, respectively. The system studied herein is a colloidal suspension of destabilized polystyrene-latex nanospheres, but the ubiquitous nature of fractal aggregates extends our implications to the aerosol phase as well. The data show that backscattering from fractal aggregates is not a function of angle but is a function of time which parameterizes the extent of aggregation. The backscattered intensity initially increases with time, but eventually levels off while the system continues to aggregate.

9AP.10

Shape and Structure of Alkane+CO₂ Multicomponent Particles from FTIR Measurements. YENSIL PARK, Ruth Signorell, Barbara Wyslouzil, *The Ohio State University*

The shape and structure of particles can affect their growth as well as their aerodynamic and optical properties. When the particles are comprised of small molecules with relatively strong transition dipoles ($> \sim 0.1$ D), the shape and structure of the particles can affect the shape of the IR spectra. A specific example is the antisymmetric stretching vibration of CO₂. Here, we investigate the structure of multicomponent nanoparticles comprised of n-alkane and CO₂. The particles are formed by homogeneous and heterogeneous condensation in a supersonic Laval nozzle. In total, two different n-alkanes, pentane and hexane, were investigated at three different flow rate conditions (LF, MF, and HF) with ~ 12 % of CO₂ and the carrier gas, Ar. The particles and the gas mixture were characterized using pressure trace measurements (PTM), small angle x-ray scattering (SAXS), and Fourier transform infrared spectroscopy (FTIR), and based on an integrated analysis of the experimental results, a few possible shapes and structures were determined. Exciton calculations were then performed to confirm and refine these structures. For the LF_{C₅}+CO₂ and MF_{C₅}+CO₂ conditions, experimental IR spectra suggest a core-shell structure where the core is the mixture of pentane and CO₂ and the shell is pure CO₂. For the LF_{C₆}+CO₂ and MF_{C₆}+CO₂ cases, both lens-on-sphere and core-shell are possible. The former corresponds to a hexane lens on a truncated cube shaped CO₂ "sphere", and the latter corresponds to a hexane core and thick CO₂ shell. The shape of the IR spectra in the HF_{C₆}+CO₂ case is quite different from the other cases, and is most consistent with elongated CO₂ domains on the hexane particles.

9AP.11**Size, Structure, and Phase of Carbon Dioxide Aerosols Formed by Homogeneous Nucleation in a Supersonic Laval Nozzle.**

KAYANE DINGILIAN, Ruth Signorell, Barbara Wyslouzil, *The Ohio State University*

Supersonic separation is a promising technology that has been proposed for carbon capture. Twister BV and TransLang Technologies Ltd. have already integrated this method into field plants for the large-scale separation of hydrocarbons from natural gas. Understanding and characterizing carbon dioxide particle formation and growth is crucial for the successful adaptation of supersonic separation to the removal of carbon dioxide (CO₂) from exhaust gas. Previously, we used position-resolved pressure trace measurements (PTM) and small angle x-ray scattering (SAXS) to characterize the onset conditions for homogeneous carbon dioxide nucleation and to calculate experimental nucleation and growth rates. Particle sizes and number densities were obtained by fitting the SAXS spectra assuming the aerosol is a polydisperse collection of spheres. Here, we combine the results from SAXS with new data from Fourier transform infrared (FTIR) spectroscopy measurements to characterize the structure and shape of the condensed CO₂ particles. Position-resolved FTIR spectroscopy measurements are performed over the range of 1000 to 4000 cm⁻¹ with particular focus on the ν₃ fundamental vibration peak near 2350 cm⁻¹. Spectra from measurements on a system of CO₂ expanding from a stagnation pressure of 7327 Pa suggest the transition from the vapor to condensed phase is dominated by direct deposition of solid CO₂. As the condensed phase grows, the ν₃ peak shifts to 2359 cm⁻¹ with a shoulder at 2360 cm⁻¹. Ongoing collaborations with molecular dynamics and spectroscopy simulation groups provide insight on the shape and structure of the CO₂ particles as they evolve from the smallest particles we can detect to the final size at the nozzle exit.

9AP.12**A General Description of Light Scattering by Particles of Arbitrary Size, Shape and Refractive Index.** JUSTIN

MAUGHAN, Christopher Sorensen, *Kansas State University*

The orientationally averaged light scattered by a variety of shapes including spheres, spheroids, cylinders, hexagonal columns, rectangular columns, and Gaussian random spheres has been calculated. Various numerical techniques based on the Mie equations, T-Matrix, ray tracing and the discrete dipole approximation were used to calculate the orientationally averaged scattering. We show that when the orientationally averaged scattering is normalized by the Rayleigh differential cross section, the scattering develops from the three-dimensional diffraction limit or Rayleigh Debye Gans limit to the two-dimensional diffraction limit. Furthermore, it will be shown that despite having different shapes, refractive indices, aspect ratios and sizes there is a quasi-universality of the light scattered by particles with the same internal coupling parameter.

9AP.13

Variations of New Particle Formation (NPF) Events during 2016-2018 in the Arctic Area (Ny-Alesund, Norway). HAEBUM LEE, Young-Jun Yoon, Kihong Park, *Gwangju Institute of Science and Technology*

The Arctic area includes snow-covered land, sea ice, and ocean diversely affecting the Arctic climate system, and is so vulnerable to global climate change (M.O. Jeffries, & J Richter-Menge, 2012). Also, nanoparticles can grow up to sizes which have potential to become the CCN with the high population, affecting cloud properties. Thus, it is essential to understand major processes, leading to form nanoparticles in the Arctic atmosphere. The Arctic haze was observed in spring with increased pollutants transported from continents (Rahn and Shaw, 1977), and NPF events were often observed in summer (J Heintzenberg, et al., 2017). In this study, particle number size distribution in the size range of 3 nm to 60 nm was measured by a scanning mobility particle sizer (SMPS), which includes a nano-differential mobility analyzer (nano-DMA) (3081, TSI, USA) and an ultrafine condensation particle counter (UCPC) (3776, TSI, USA), to investigate NPF events during 2016 to 2018 at the Zeppelin laboratory (78.91° N, 11.88° E) in Ny-Alesund, Norway.

The highest particle number concentration for N(3-20 nm) and N(20-60 nm) were found in summer while both were the lowest in winter. Five distinct clusters were found, and the mode diameters of clusters were found to be 3.5 nm (cluster 1), 5 nm (cluster 2), 10 nm (cluster 3), 20 nm (cluster 4), and 40 nm (cluster 5), respectively. The fractions of clusters 1 and 2 significantly decreased in summer while the fractions of clusters 4 and 5 increased. Total 115 NPF event days during measurement period were counted (~ 16 % per year), and the highest percentage of NPF event days was observed in May, June, July, and August. In April, the NPF starting time was 9:00, and gradually increased up to 12:00 in July. The NPF duration time was around 5-6 hours on average, and higher in May-September than April and October. The overall average of GR appeared 1.56 ± 0.77 nm/h, and it was shown that the mean and median values were 1.65 nm/h and 1.54 nm/h, respectively.

9AP.14

Homogeneous Ice Nucleation From Supercooled Nanodroplets ~230 K. TONG SUN, Barbara Wyslouzil, *The Ohio State University*

Homogeneous ice nucleation within highly supercooled water droplets ($160 \text{ K} < T < 235 \text{ K}$) is a nonequilibrium phenomenon of ongoing interest in part because of the insight it provides into the phase behavior of water under extreme conditions. The reported ice nucleation rates ~230 K remain controversial: rates reported in droplets with radii ~10nm at temperatures of ~225K are ~9 orders of magnitude higher than those reported in 10 μm droplets at ~227K. Here, we seek to make droplets with radii around 20 nm and freeze them at higher temperature in order to fill the gap between the previous studies. To increase the size of the droplets, we use a shaped supersonic nozzle to condense water vapor and then freeze the supercooled droplets. The special design of the nozzle allows us to produce droplets with radii around 20 nm and the extended expansion region length makes it possible for the droplets to freeze at ~230K. A movable probe is used to measure the position-resolved pressures and by integrating the adiabatic flow equations, the temperature, density, velocity of the gas mixture, effective area ratio of the nozzle and the mass fraction of the condensate are obtained. By recording the peak position and intensity changes, Fourier Transform Infrared spectroscopy provides the onset conditions for ice nucleation and fractions of the aerosol that has frozen. Small Angle X-ray Scattering characterizes the aerosol size and number density. The behavior of ice nucleation ~230 K is elucidated based on these thorough characterizations. The comparison of the experimental data with the rates given by classic nucleation theory further illustrates the effect of the Laplace pressure on ice nucleation rates of nano-sized droplets.

9AP.15**Simulation and Evaluation of the Effectiveness of House Sheltering from the Perspective of the Penetration Factor.**

WENLU WANG, Nobuyuki Kato, Shigeru Kimoto, Yasuto Matsui, Minoru Yoneda, *Kyoto University*

When air pollution incidents or extreme weather occurs, outdoor sources of pollutants penetrate into houses, negatively affecting indoor air quality and endangering human health. Using the most common housing design, this study simulates the process of particles passing through cracks of a building from the outside under air pollution conditions. The effectiveness of house sheltering was assessed by focusing on the charging effect and particle diameter. A high penetration factor corresponds to a high particle flow concentration. An air exchange rate higher than 1.20 h^{-1} can effectively remove indoor particles (ultra-fine particles and fine particles less than 500 nm in diameter), but it also increases the penetration factor and the risk of a large number of outdoor particles entering indoors. Uncharged particles are more susceptible than neutralized ones to external forces provided by the ventilation system.

Acknowledgments: This work was financially supported by the Nuclear Regulation Authority (NRA) of Japan and the Japan Atomic Energy Agency (JAEA).

9AP.18**Black Metal Nanoparticles from Abrasion Processes in Our Everyday Lives: Bicycle Chains, Rock Climbing Ropes, and Motor Oil.** HANS MOOSMULLER, Ramesh Giri, Matthew Berg, Christopher Sorensen, *Desert Research Institute*

Black carbon is often thought to dominate particle light absorption due to its high bulk absorption coefficient. Here, we examine some manifestations of small black particles in our everyday lives including the ubiquitous blackening of bicycle chains, climbing ropes, and motor oil. We present experimental and theoretical evidence that this blackening is caused by black metal nanoparticles, not by black carbon. While metals are commonly thought of being highly reflective, this is only true if the imaginary part of the refractive index and its product with the size parameter x are both larger than ~ 3 (Sorensen et al., 2019); this is generally true for metals in our everyday experience. However, for metallic nanoparticles, the second condition is generally not fulfilled and metal particles become black and highly absorbing with a very low single scattering albedo (Moosmüller and Sorensen, 2018) and with an appearance resembling that of black carbon.

References:

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- [2] Moosmüller, H. and C. M. Sorensen (2018). Small and Large Particle Limits of Single Scattering Albedo for Homogeneous, Spherical Particles. *J. Quant. Spectrosc. Radiat. Transfer*, 204, 250-255, <https://doi.org/10.1016/j.jqsrt.2017.09.029>.

9AP.19

A Hybrid Continuum-Molecular Dynamics Flux Matching Calculation Method for Collision Rate Coefficients. TOMOYA TAMADATE, Christopher Hogan Jr., Hidenori Higashi, Yoshio Otani, Takafumi Seto, *Kanazawa University*

Particle-ion or ion-ion collision in the gas phase, i.e. charging processes, are important in a variety of aerosol technologies and measurement systems. A central challenge in aerosol science is hence the accurate calculation of charging rates, defined as the collision rates between particles and ions, and recombination rates, which are ion-ion collision rates. Such collision rate coefficients are challenging to calculate in aerosols because neither continuum or free molecular approaches are strictly applicable. Fuchs's limiting sphere model (Fuchs, 1963) is normally adapted to calculate collision rate coefficients for charging. However, Fuchs' theory has a number of shortcomings; the theory assumes that when the colliding species are sufficiently far from one another (outside the limiting sphere), continuum equations of motion are valid and then inside the limiting sphere, motion is free molecular. Filippov (1993) noted that Fuchs's model could be made much more general by choosing a sufficiently large critical distance beyond which continuum equations apply, and then noting that collisions with gas molecules inside limiting sphere should be accounted for. Limitations in computational speed at the time prevented complete implementation of Filippov's approach. However, vastly increased computational power now enables application of this method, hence we have developed a hybrid continuum-molecular dynamics approach for collision rate calculations, where continuum equations describe motion for species farther apart than a prescribed sphere radius, and molecular dynamics calculations with LAMMPS are used to monitor motion inside the sphere radius. We show that the method is general, and enables all atom based models to be employed in charging rate calculations, along with a wide variety of transition regime rate calculations.

9AS.1

Laboratory and Field Evaluation of Real-time and Near Real-time PM_{2.5} Smoke Monitors. HANS MOOSMULLER, Ahmed Mehadi, David Campbell, Walter Ham, Donald Schweizer, Leland Tarnay, Julie Hunter, *Desert Research Institute*

Increases in wildfire frequency and intensity and a longer fire season in the western USA are resulting in a significant increase in air pollution, including PM_{2.5} concentrations that pose significant health risks to nearby communities. During wildfires, government agencies monitor PM_{2.5} mass concentrations providing information and actions needed to protect affected communities; this requires continuously measuring instruments. This study assessed the performance of seven candidate instruments: (1) Met One Environmental beta attenuation monitor (EBAM), (2) Met One ES model 642, (3) Grimm Environmental Dust Monitor 164 (EDM), (4) Thermo ADR 1500 (ADR), (5) TSI DRX model 8543 (DRX), (6) Dylos 1700, and (7) Purple Air II in comparison with a BAM 1020 (BAM) reference instrument. With the exception of the EBAM, all candidates use light scattering to determine PM_{2.5} mass concentrations. Our comparison study included environmental chamber and field components, with two of each candidate instrument operating next to the reference instrument. The chamber component involved six days of comparisons for biomass combustion emissions. The field component involved operating all instruments in an air monitoring station for 39.5 days with hourly average relative humidity (RH) ranging from 19% to 98%. Goals were to assess instrument precision and accuracy and effects of RH, elemental (EC), and organic carbon (OC) concentrations. All replicate candidate instruments showed high hourly correlations ($R^2 \geq 0.80$) and higher daily average correlations ($R^2 \geq 0.90$), where all instruments correlated well ($R^2 \geq 0.80$) with the reference. The DRX and Purple Air overestimated PM_{2.5} mass concentrations by a factor of ~two. Differences between candidates and reference were more pronounced at higher PM_{2.5} concentrations. All optical instruments were affected by high RH and by the EC/OC ratio. Equations to convert candidate instruments data to FEM BAM type data were developed to enhance usability of data from candidate instruments.

9AS.2

Low-cost Sensor Packages in Parking Garages to Determine Emission Factors and Assess the Relative Importance of Cold Start Operation on Air Quality. BINGQI LIU, Katia Cantu Flores, Sakshi Jain, Mrinmoy Chakraborty, Naomi Zimmerman, *University of British Columbia*

Traditionally, measurements of vehicle emissions have relied on reference-grade instruments whose complex operation and high cost have limited their deployment in real-world environments. With new low-cost sensing technologies, continuous measurements of vehicle emissions are now possible in traffic-impacted real-world environments, such as parking garages, where exhaust from on-board engines at low-speed, idle, and cold-start operation can severely affect the air quality.

In this study, the Sensit Real-time, Affordable, Multi-Pollutant (RAMP) monitor for measuring PM_{2.5}, NO, NO₂, CO₂, O₃ and CO was deployed in six locations across three parking garages on the UBC Vancouver campus from April – August 2019. One sensor was located at the entrance to the parking garage, and the other in the main vehicle corridor furthest from the parking garage exterior where ventilation is poorest. The RAMP sensors measured the air quality every 10 seconds, providing a high time-resolution dataset of the real-world concentration of traffic-related air pollutants. In addition to the air pollution data, UBC Parking Services provided vehicle count and timing information to better associate pollutant spikes with vehicle patterns.

The integrated pollutant and CO₂ signals have been used to develop fuel-based emission factors for the five pollutants measured by the RAMP monitors and to measure the relative impact of cold-start. Individual plumes as well as hourly average pollutant:CO₂ ratios are being used to develop these emission factors. Additionally, diurnal pollutant patterns within the garages are being used to target times for increased ventilation in the garages to improve air quality and decrease human exposure. Sensor data is also displayed on a UBC hosted website to encourage motorists to consider their air quality and climate impacts of driving to campus vs taking public transit or bicycling.

9AS.3

From Building Blocks to Building Air-Quality Sensors, Air-Quality Estimates and Citizen Scientists. KERRY KELLY, James Moore, Wei Xing, Matt Dailey, Katrina Le, Tofigh Sayahi, Tom Becnel, Pascal Goffin, Miriah Meyer, Pierre-Emanuel Gaillardon, Deborah Burney-Sigman, Jason Weise, Ross Whitaker, Anthony Butterfield, *University of Utah*

The Salt Lake Valley periodically experiences the highest levels of fine particulate matter (PM_{2.5}) in the nation. We have been engaging community members and students across Utah's Salt Lake Valley as citizen scientists who work in partnership with an interdisciplinary team of researchers to create a distributed online network of approximately 100 low-cost, air-quality sensors. Our website dynamically provides visualizations of neighborhood-scale PM_{2.5} concentrations. Thus far, this network has generated a rich set of PM measurements, capturing several severe PM episodes resulting from persistent cold air pools, fireworks, wildfires and dust events. We highlight how we calibrate our low-cost PM sensors, exclude suspect readings, and dynamically estimate PM levels (as well as uncertainty) with a Gaussian process model. The results illustrate dramatic geospatial differences in PM_{2.5} concentration during some of these episodes that would not have been observed from the regulatory monitors alone. Through outreach efforts to local schools, we also engaged students as citizen scientists through activities that: (1) allow them to build their own light-scattering based PM sensor from building blocks and simple electronics; (2) train them on how to be good sensor hosts; and (3) help them make sense of real-world data. Citizen science poses a number of challenges, and we describe some of these and strategies to address them. Our teacher surveys and student feedback suggest that these modules are highly engaging and effective for improving students' awareness of air quality, the principles behind light-scattering based sensors and the geospatial and temporal variations in PM_{2.5} levels during a variety of pollution episodes.

K. Kelly and P.-E. Gaillardon have an interest in the company Tetrad: Sensor Network Solutions, which commercializes solutions for environmental monitoring.

9AS.4

Spatiotemporal Mapping of Ultrafine Particles in Buildings with Low-Cost Sensing Networks. DANIELLE WAGNER, Brandon E. Boor, *Purdue University*

A significant fraction of human exposure to ultrafine particles (UFPs) occurs indoors. UFP number concentrations cannot be inferred from $PM_{2.5}$ mass concentration data from low-cost optical particle sensors. Traditionally, UFP measurements have been dependent on expensive aerosol instrumentation. Advances in the electrical detection of UFPs has made it possible to deploy low-cost UFP sensing networks in different environments. The integration of UFP sensing networks with building systems provides a unique opportunity to determine optimal building ventilation and filtration control strategies to reduce occupant UFP exposures. The objective of this study is to investigate spatiotemporal trends in UFP concentrations throughout an office building and its HVAC system through deployment of a low-cost UFP sensing network.

An eight-month measurement campaign was performed at the Herrick Living Laboratories at Purdue University, which are four modern open-plan offices with precisely controlled HVAC systems. A distributed UFP sensing network was established in an office and HVAC system with four portable electrical particle charging (EPC)-based UFP sensors. Sensing nodes included: indoor air (IA), outdoor air duct (OA), supply air duct: pre-filter (SAPR), and supply air duct: post-filter (SAPO). The EPC-based UFP sensors measured total particle number and surface area concentrations from 10 to 2,500 nm at one-second time-resolution via sensitive electrometers and were calibrated against a water-based condensation particle counter. A state-of-the-art building automation system monitored and controlled the HVAC system. Variable ventilation modes were implemented to evaluate the response of the UFP sensing network to dynamically changing conditions.

The creation of a building-scale low-cost UFP sensing network identified significant spatiotemporal trends in UFP number and surface area concentrations in an occupied office and its HVAC system. Temporal patterns in UFPs at all four nodes were strongly influenced by ambient air pollution, indoor sources, and ventilation mode. The relative magnitude of UFPs at the IA and OA nodes varied depending on the strength of indoor and outdoor UFP sources. SAPR remained > SAPO, providing insight into *in situ* UFP removal via HVAC filtration. The UFP data will be integrated with material balance models to infer time-dependent UFP source and loss processes, as well as daily-integrated occupant exposures and I/O ratios. This pilot study can inform the development of real-time UFP-based ventilation control for commercial buildings.

9AS.5

Using Mini-PEMS to Monitor Motor Vehicle Exhaust PM. Diep Vu, Joseph Szente, Michael Loos, MATTI MARICQ, *Ford Motor Co.*

As regulations evolve to require cleaner motor vehicle exhaust, attention is turning to ensuring these are not only met in certification tests but also in real world driving. The failure in Europe of diesel vehicles meeting EU6 NOx standards to exhibit comparable emissions in real world driving precipitated development of "read driving emissions" testing, in which emissions are recorded using portable emissions measurement systems (PEMS) during on-road tests. Similar regulations are being adopted in other parts of the world. The US already has in place "not to exceed" regulations for on road testing of in-use heavy duty vehicles. These regulations extend as well to particle emissions.

On-road regulations extend the testing burden during engine and exhaust aftertreatment development in two ways: First, more emissions testing is required to cover the large variability of on-road driving conditions, e.g., speed, load, grade, temperature, altitude, etc. Second, additional testing equipment, namely PEMS, is required. Commercial PEMS that meet regulatory requirements are bulky, costly, and difficult to operate, further exacerbating the testing burden.

The recent development of mini-PEMS offers an alternative. These are smaller, relatively inexpensive, sensor based systems. The tradeoff is that they generally lack the stability and accuracy of the full PEMS. However, they can still perform a useful function as a survey tool to determine engine / driving conditions that lead to undesired emissions levels, after which these situations can be studied more accurately and in more detail in laboratory testing.

The present work examines four commercial mini-PEMS employing four different PM sensing technologies for their ability to detect PM emissions from current gasoline direct injection vehicles. PM is a complex substance that is regulated differently in various parts of the world, for example by total PM mass in the US and by solid particle number in the EU. We find that the mini-PEMS have trouble providing accurate absolute PM mass or solid particle number readings owing to the difficulty in converting their sensor response to number or mass units. But, they provide good qualitative capability for detecting PM emissions events and, thus, can provide useful on-road survey data.

9AS.6

Design and Evaluation of a Portable PM Monitor Featuring a Low-Cost Light Scattering Sensor in Line with an Active Filter Sampler. JESSICA TRYNER, Casey Quinn, Bret Windom, John Volckens, *Colorado State University*

Fine particulate matter (PM_{2.5}) concentrations can vary by orders of magnitude over time and across microenvironments. Light scattering sensors can report real-time PM_{2.5} measurements from many locations at low cost; however, these sensors have limited accuracy. Gravimetric filter samples provide more accurate, albeit time-integrated, measurements that can be used to correct light scattering sensor data. Correction of light scattering sensor data is key; for example, gravimetric correction factors for nephelometer-derived PM_{2.5} concentrations varied by a factor of three in two recent studies: one involving personal sampling of adults commuting two and from work in Colorado and one involving stationary sampling in Honduran homes with biomass-fueled cooking stoves.

This work describes a new portable PM_{2.5} monitor that features a low-cost light scattering sensor in-line with an active filter sampler. Laboratory tests were used to determine (1) the accuracy and precision of PM_{2.5} concentrations derived from the filter sample and (2) gravimetric correction factors for the response of the low-cost sensor to ammonium sulfate, Arizona road dust, urban PM, and match smoke. Filter samples collected at 0.25 L·min⁻¹ (n = 12; 4 tests with 3 monitors) had a mean bias of -10% (relative to a TEOM). The relative standard deviation of three concurrent samples ranged from 7% to 17%. Correction factors varied from 1.2 to 6.3 depending on the test aerosol and the individual monitor. Gravimetric correction improved the accuracy and precision of 1-hour average concentrations reported by the light scattering sensor. The monitor was also deployed in a week-long field experiment to study sources and concentrations of residential air pollution. Field data were used to identify: (1) pollution events resulting from occupant cooking and heating activities and (2) variations in the number of air changes per hour inside the residence.

9AS.8

Evaluations of Three Commercially Available Indoor PM_{2.5} Monitors. MISTI ZAMORA, Kirsten Koehler, *Johns Hopkins Bloomberg School of Public Health*

The availability of low-cost monitors marketed for use in personal homes has increased rapidly over the past few years due to the advancement of sensing technologies and the rise of citizen science. The user-friendly packages can make them appealing for use in indoor exposure projects, but a rigorous scientific evaluation has not been conducted for many monitors on the open market, which leads to uncertainty about the validity of the data. We evaluated six monitors (two Air Visual Pros, two Speck sensors, and two Airthinx) over a one-year period in a residential setting. All of the selected monitors measure PM_{2.5} mass concentration, temperature, relative humidity, store data internally, and have a way to indicate poor air quality to the consumer. Two units of each type of monitor were evaluated to determine the precision between units, and a personal DataRAM (pDR-1200) with a filter was placed in the home for about 20% of the sampling period (e.g., about a week each month) to evaluate the accuracy over time. The average PM_{2.5} mass concentrations from the periods of colocation with the pDR were 8.64 µg/m³ for the pDR-Filter, 9.66 µg/m³ for the pDR-Nephelometer, 8.00 and 8.02 µg/m³ for the Air Visual Pro units, 13.02 and 21.28 µg/m³ for the Speck units, and 12.05 and 10.36 µg/m³ for the Airthinx units. The Air Visual Pro exhibited the best accuracy at 88%, which was comparable to the nephelometric component of the pDR compared to the filter weight (also 88%). The accuracy of the Speck and Airthinx were -207 and 43%, respectively. The precisions of the Air Visual Pro, Speck, and Airthinx were 0.11, 0.38, and 0.18, respectively. For comparison, ambient regulatory instruments must be below 0.10. The Pearson correlation coefficients (R²) between units of the same type were 0.99, 0.52, and 0.91 for the Air Visual Pro, Speck, and Airthinx, respectively. The R² between the units and the pDR were 0.98, 0.45, and 0.91 for the Air Visual Pro, Speck, and Airthinx, respectively. Overall, the reliability of these types of monitors is strongly dependent on the model, so an evaluation of each type of monitor is essential before the data can be used to assess residential exposures.

9AS.9

Towards a Highly-Integrated Low-Cost PM Sensor. PAUL MAIERHOFER, Georg Röhrer, Jaka Pribošek, Gernot Fasching, Anderson Singulani, Harald Etschmaier, Martin Kraft, Alexander Bergmann, *Graz University of Technology*

Increasing awareness about the adverse health effects of particles in the air and stricter regulations on the part of the legislation lead to greater demands on the measurement and monitoring of air quality with respect to particle concentration. Up to now, a close-meshed and wide-area monitoring has failed due to the size, usability and cost of currently available sensors.

We show our approach to build a highly integrated, cost-effective, maintenance-free and easy-to-use particle sensor for mobile applications. While space is limited, the necessary complexity of a total miniaturized sensor system is still similar to its handheld counterparts. Optical elements for the light scattering based sensor element, a suitable flow path for the ambient air, a pump to cause the airflow and the electronics – all within a package of roughly $12 \times 9 \times 2 \text{ mm}^3$. We show our design of the sensor including the package with an integrated impactor, and the optical sensor element consisting of a VCSEL as a light source, a beam guiding structure, a photodiode, and a beam trap. Microfluidic considerations and simulations lead to an optimized interaction of the flow path with the optical elements. The package itself is coated with a highly light absorbing material in order to minimize stray light effects and to enhance the capability of the light trap. This minimization of stray light is a crucial step towards a functional sensor, as the signal scattered from the particles has to dominate over the stray light from other surfaces. We also show the concept for integrating a micro-pump in the system as well as an overview of selected challenges along the way such as the manufacturing of the prototypes. First measurement results utilizing PSL spheres of various sizes will be shown to evaluate the capabilities of the sensor.

9AS.10

Spark-Plug Sized Automotive Exhaust Aerosol Sensors for Emission Monitoring and On-Board Diagnostics. VINAY PREMNATH, Imad Abdul-Khalek, *Southwest Research Institute*

The California Air Resources Board has instituted requirements for on-board diagnostics (OBD) that make spark-plug sized particulate matter (PM) sensors critical components of vehicle exhaust aftertreatment systems. These sensors are typically used on diesel engine platforms to monitor health of diesel particle filters. While these sensors are currently utilized for OBD, there is tremendous interest globally among regulators and engine manufacturers to use such sensors for emission monitoring wherein real-time sensor signal would be broadcast to the cloud. Such a large database would assist regulators, air quality, climate and health researchers.

Prior to being widely adopted, in-depth knowledge of the performance of such sensors is important. This work reviews the state-of-the-art in automotive exhaust aerosol sensing and discusses the experimental evaluation of these technologies. Experimental results from two campaigns will be discussed. The first campaign focused on evaluating performance of real-time and accumulation-type sensors as a function of exhaust PM concentration, size distribution, velocity and temperature. A 1998 model year (MY) heavy-duty diesel engine was used. The second campaign involved evaluation of a real-time sensing technology using a 2011 MY heavy-duty diesel engine equipped with a complete aftertreatment package. Sensors were tested under both, steady-state as well as transient engine operating conditions. During both campaigns, aerosol sensors were benchmarked against real-time laboratory instrumentation. AVL micro-soot sensor was used for soot mass measurement and TSI engine exhaust particle sizer coupled with SwRI's solid particle sampling system was used for solid particle number and size measurement. Accuracy, variability and lower detection capability of sensors were examined.

This work sheds some light on the state of automotive exhaust aerosol sensing and outlines some steps required to develop a reliable sensing technology that can be used for emission monitoring.

9AS.11

A Physical-property Based Method to Characterize Low-cost Sensor. MEILU HE, Nueraili Kuerbanjiang, Suresh Dhaniyala, *Clarkson University*

Low-cost sensors, based on optical sensing of particles, have become very popular for air pollutant monitoring in indoor and outdoor environments. While we have a good understanding of the general physics underpinning these sensors, we lack a direct understanding of their specific response characteristics as a function of particle type, size, concentration, etc. Most applications currently rely on machine learning models built with field data at a certain location and time period. But outside the calibration region and time period, significant errors could be resulted. Here, we study a popular low-cost sensor – Plantower PMS5003 – to determine the detection characteristics of its different channels as a function of particle properties. The sensor signals were obtained for a range of test particle properties and the measurements were compared to research-grade instruments, and the signals were then analyzed to obtain the sensor channel transfer functions. The sensor transfer function allows us to understand the particle size- and composition-dependence of the signal in the different channels and helps in improving the accuracy of measurements made with these sensors. We will present our experimental approach, analytical techniques, and the obtained sensor transfer functions in our presentation.

9AS.12

Correlation Measurements of Indoor and Outdoor Particulate Matter Air Quality Using Low-Cost Air Pollution Sensors at a Freeway Site in Southern California. DANIEL B. CURTIS, Linh K. Luu, Brian M. Chavez, Karen E. McReynolds, *California State University, Fullerton*

The use of low-cost air pollution sensors is increasing rapidly due to their low-cost, small size, high time resolution, reliability and robustness, low power requirements, and ability to upload data online automatically for display on online maps available to the public. Although scientific-grade instruments provide high mass resolution and accurate measurements of pollutants, their bulk, complexity, and high cost make them impractical for large-scale projects. Low-cost air monitors therefore provide an opportunity to collect data in a large range of locations simultaneously for comparison. This study involved an evaluation of low-cost sensors to measure the particulate matter air quality indoors and outdoors under relatively non-polluted and polluted conditions near a freeway location in Southern California, USA. A total of three PurpleAir sensors (each containing two Plantower PMS5003 modules) were deployed on the adjacent campuses of California State University, Fullerton (CSUF) and Hope International University (HIU). One of the sensors was located indoors, while two sensors were located outdoors, allowing for a comparison between the indoor and outdoor air quality over a period of several months in 2018-2019. In this case, the number and mass concentrations of $PM_{2.5}$, $PM_{1.0}$, and PM_{10} were all lower indoors compared to outdoors, but the differences between indoor and outdoor air quality varied with particle size. Additionally, the measurements show a strong correlation between outdoor and indoor air pollution, indicating that outdoor aerosol particles are a significant source of indoor air pollution at this site. The results of this study indicate that low-cost sensors can be used to make comparison measurements of indoor and outdoor air quality. Overall, low-cost air sensors provide a unique platform for making comparison measurements across multiple locations cheaply, with high spatial and time resolution.

9AS.13

Calibration of C-RUV Aerosol Acidity Measurement Using Two Inorganic Thermodynamic Models and Its Application to Field Data. SHIQI SUN, Myoseon Jang, Sanghee Han, Chufan Zhou, Ryan Winslow, *University of Florida*

Despite numerous studies that report the association of aerosol acidity with health effects of particulates and aerosol chemistry, the accuracy in measuring aerosol acidity is uncertain. In a typical aerosol sample applied to a measurement of the concentration of proton ($[H^+]$ mol/L of aerosol), the collected aerosol is extracted with water to analyze ion species with ion chromatography (IC). Then, an inorganic thermodynamic model with IC data determines $[H^+]$ in aerosol. However, non-ideality associated with activity coefficients of ionic species in aerosol is dissimilar from that in dilute aqueous solution. Most data reported in the literatures are produced in highly humid aerosol or highly acidic sulfate-rich aerosol. Therefore, the prediction of $[H^+]$ by inorganic thermodynamic models is also hampered by the uncertainty in database. 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) by avoiding the use of solvents. In this study, $[H^+]$ measurement by the C-RUV is calibrated for sulfate-rich inorganic aerosols where the uncertainty in inorganic thermodynamic models is low to predict $[H^+]$. The two calibration equations for C-RUV data are obtained using two different inorganic thermodynamic models, E-AIM and ISORROPIA. Then, calibration equations are extrapolated to ammonia-rich aerosols where the thermodynamic models poorly perform. $[H^+]$ determined using C-RUV data is deviated from the prediction using both models, although less with E-AIM. C-RUV is also applied to ambient data collected in Gainesville, Florida. Overall, aerosol acidity is high ($pH < 1$) in summer while it is low ($1 > pH > 3$) in winter due to the condensation of ammonia gas to aerosol at low temperature.

9AS.14

Application and Use of Low-cost Sensors for Air Quality Monitoring. YI LI, Houxin Cui, Mengxian Wu, Zhanbang Feng, *SailBri Cooper Inc*

Low-cost air quality sensors have attracted increasing attention in recent years due to their advantages over conventional methods, such as low power requirements, easy installation, and deployability in large numbers to cover large spatial areas. However, they also face many technical challenges regarding data quality, including signal drift, temperature/humidity effect, cross-interference, etc. To mitigate such issues and build a robust sensor-based system, a four-stage calibration quality control system is implemented, including standard material calibration, simulated environmental calibration, combined supervision calibration, and transfer calibration.

During standard material calibration, each individual sensor is screened for quality assurance by testing its response to known concentrations of standard gases of criteria air pollutants (SO_2 , NO_2 , CO , and O_3). Then, the selected sensors are assembled into "sensor node" to measure the multiple pollutants simultaneously. These sensor nodes are then put in a control chamber to perform simulated environmental calibration. Standard gases and particulate matters are injected into the chamber simultaneously to simulate a wide range of ambient conditions by controlling temperature and humidity. Machine learning and neural-networking algorithms are applied to characterize sensor response. Next, the sensor nodes are installed outdoor with a Federal Reference Method (FEM) monitor in close vicinity to conduct in-field combined supervision calibration. Since the real ambient atmosphere is more complicated than the controlled chamber conditions, the FEM data is used to train the algorithms for improved sensor response. In regions without FEM nearby, the transfer calibration is implemented using mobile or portable equipment to optimize the calibration parameters.

The result shows that (1) after standard material and simulated environmental calibration, the correlation between sensors and FEM measurements increased from 0.4-0.6 to over 0.95; (2) after adaptive learning through in-field combined supervision and/or transfer calibration, the correlation between sensor and FEM improved from 0.6-0.75 to over 0.85. Over 10,000 sensor nodes (over 60,000 single sensors) calibrated through this four-stage calibration system have been successfully deployed in more than 80 cities across China and are currently being used in air quality monitoring for environmental management, research, and consulting. Recently, two sensors also show a steady performance during the wildfire season in the U.S.

9AS.15

Real-time Sampling of Total Biogenic Volatile Organic Compounds Using a Compact, Portable Photoionization Detector. MATTHEW STEWART, Jianhuai Ye, Tianning Zhao, Karena McKinney, Scot T. Martin, *Harvard University*

The biosphere emits a complex mixture of volatile organic compounds (VOCs) of varying reactivities into the atmosphere. Many of these are highly reactive components that can significantly influence the overall chemical reactivity of the atmosphere even at very low (sub-ppbv) concentrations. VOC concentrations also vary markedly over small spatial (10's to 100's of meters) and time (seconds to minutes) scales. In order to fully quantify VOC emissions and chemistry, measurements that capture this spatial and temporal variability are needed. Traditional techniques for measuring VOCs have been limited by several factors, including high cost, low portability, and, in some cases, slow response time, constraining their ability to fully capture the spatial variation in VOC concentrations in particular. In addition, while measurements of speciated VOCs are valuable for understanding the relationship between ecosystem types and emissions or detailed chemical mechanisms, measures of total VOCs and their reactivity would be valuable in helping to close the gap between the sum of observed individual concentrations and total reactivity that has been observed in some studies.

In this work, we present a method for estimating ambient outdoor concentrations of total biogenic VOCs, a proxy for the collective behavior of VOCs and their net effects on oxidation capacity, in real time using a photoionization detector (PID). PIDs are a mature sensor technology commonly used as detectors within gas chromatograms and for indoor air quality monitoring, but several challenges, such as sensitivity to temperature, humidity, chemical species, and its inherent non-selectivity, have hindered their implementation for ambient outdoor sampling of VOCs. Through a combination of laboratory and chamber studies, robust calibration procedures using isoprene, α -pinene, and β -caryophyllene were developed for estimating total biogenic VOCs using high-sensitivity commercial PIDs. These procedures manage the humidity and temperature sensitivities typically associated with PIDs to provide accurate and repeatable measurements when compared to a proton transfer reaction mass spectrometer.

Field tests to validate the accuracy of measured total VOC concentrations are planned in temperate and tropical forests, with the eventual aim of performing real-time aerial measurements using civilian unmanned aerial vehicles. PIDs offer a portable means to obtain measurements of total biogenic VOCs with high time resolution, which provide atmospheric scientists with new ways to help to constrain VOC emission estimates, as well as to attribute unexplained reactivity to highly reactive organic species.

9AS.16

Field Evaluation and Calibration of a Six-Parameter Low-Cost Sensor System in Northwestern and Southeastern US. Yi Li, HAOFEI YU, Zack Fregin, *SailBri Cooper Inc*

The fast-evolving low-cost sensor systems are enabling new possibilities for detailed characterization of the spatial distributions of air pollution concentrations. In this study, we evaluated the performances of the SCI-608 sensor system at two locations in the US with distinct climate conditions: Portland, OR and Orlando, FL. This integrated system simultaneously measures ambient concentrations of six common air pollutants: CO, NO₂, SO₂, O₃, PM_{2.5}, and PM₁₀. In addition to compare raw sensor measurement data with data as measured by reference instruments, we also performed sensor calibrations using multiple methods including the build-in multiple regression method, and machine learning approaches. Preliminary results suggest the SCI-608 sensor system performed well with coefficients of determination (R²) exceed 0.9 between hourly PM_{2.5}, O₃ and CO concentrations collected from sensor and reference instruments at the Portland site. Our results substantiated the potentials for using this sensor system to construct a connected and distributed air quality monitoring network.

9AS.17**Sensitive and Selective Gas Sensing Module for Isoprene.**

TIANNING ZHAO, Jianhuai Ye, Matthew Stewart, Scot T. Martin, *Harvard University*

Interactions between the emissions and atmospheric chemistry of biogenic volatile organic compound (BVOC) pose significant impacts on regional air quality and global climate change. Emission variations from plant species are often served as an indicator in biodiversity and ecosystem functioning as response to ecosystem change and stress. Accurate emission estimates of BVOCs have been the focus of constraining the model inputs to better simulate their atmospheric fate and evaluate corresponding impacts. Isoprene, the most abundant BVOC species, is highly reactive and of great atmospheric chemistry importance. Measurements using mass spectrometers and chemi-luminescence (Fast Isoprene Sensor) approach can provide accurate data but cannot be scaled up due to limits in size and cost.

In this study, a miniature isoprene-selective sensing module is designed to be compatible with any portable platform. Through optimization of temperature cycling profile and signal processing, non-selective metal oxide semiconductors (MOS) can reach detection limit of 1 ppb isoprene with a time resolution of 1 min. Selectivity towards isoprene is realized by adsorption removal of hydrophilic species and molecular sieving for larger isoprenoids. Major interferents, such as water vapor and monoterpenes, will be removed to a negligible level. The performance is further validated with collocated PTR-MS measurements.

9AS.18**Evaluation of PurpleAir Sensors across the United States.**

KAROLINE BARKJOHN, Ian VonWald, Daniel Garver, Ryan Brown, Andrea Clements, *U.S. EPA Office of Research and Development*

PurpleAir particulate matter sensors are widely used by individuals, community groups, and other organizations including state and local air monitoring agencies; these sensors comprise a massive, global network of > 6000 sensors. Previous performance evaluations have studied PurpleAir sensors in just a few locations for short time periods and these results describing sensor behavior and data normalization may not be translatable to areas with different environmental conditions and aerosol compositions. Here, we evaluate the performance of PurpleAir sensors in comparison to collocated reference monitoring sites over time periods ranging from a few months to longer than a year. Sites are located in diverse regions across the US including Alaska, Georgia, Iowa, North Carolina, and other states. The importance of environmental conditions (i.e. temperature and relative humidity) on the accuracy and the feasibility of regional and seasonal corrections will be explored. This analysis will help to interpret PurpleAir sensor data from a wide range of environments and understand the potential of this growing low-cost sensor network to answer pressing questions about particulate exposure on personal to global scales.

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9AS.19

Low Cost Sensor Approach to Intra-Urban UFP Characterization in Austin, TX. MARK CAMPMIER, Rijul Gosar, Jing Wu, Betty Molinier, Joshua Apte, *University of Texas at Austin*

Ultrafine Particles (UFP) or particles with a diameter smaller than 100 nm have been difficult to continuously measure, characterize, and attribute to emissions sources. In addition, the influence of photonucleation in high insolation regions has required the usage of relatively expensive and challenging to maintain particle size analyzers to fully capture the nuance of UFP number concentration (PN) measured by Condensation Particle Counters (CPC). Over the course of Summer, and Fall 2018 the University of Texas at Austin conducted a citywide measurement campaign in Austin with an ensemble of sensors as part of the Center for Air, Climate, and Energy Solutions (CACES). The goal of the campaign was to evaluate the performance of the low-cost sensors, characterize intra-urban PN variation, and increase understanding of the role of local and regional emissions sources. In this study, we show that a regionally dense sensor network including packages of water-based CPCs co-located with low-cost optical PM_{2.5}, CO₂, and NO₂ sensors can effectively characterize some urban scale and neighborhood scale phenomena. Throughout the three operational phases (July 16-Aug 8, Aug 8-Aug 31, Oct 5-Nov 25) of the campaign, despite varying sensor package locations, midday peaks in PN were observed throughout the high insolation summertime. Fewer of these midday peaks were observed during phase 3, which occurred in the cooler and more nebulous autumn. During the pre-calibration phase (June 4- July 16), these peaks were observed to correlate with nucleation events measured by a co-located SMPS. Other PN peaks seemed to match expected traffic trends, with some sites experiencing only single traffic peaks (morning or evening), likely caused by wind conditions favoring a given direction of traffic. PM_{2.5} trends were relatively homogenous across the region and measurement phase, following a distinctive weekday vs weekend pattern.

9AS.20

Preliminary Assessments of Sensor Performance and Data Analysis for California Communities under a US EPA STAR Grant Project. Ashley Collier-Oxandale, VASILEIOS PAPAPOSTOLOU, Brandon Feenstra, Berj Der Boghossian, Andrea Polidori, *South Coast Air Quality Management District*

Through the US EPA STAR Grant: “Engage, Educate and Empower California Communities on the Use and Applications of Low-cost Air Monitoring Sensors”, led by AQ-SPEC at the South Coast Air Quality Management District, approximately 400 low-cost sensor devices (for both PM and PM combined with O₃ and NO₂) have been deployed across 14 California communities. The current phase of the project has involved meeting with participants to discuss their experience installing and using the sensors as well as results from a preliminary analysis of the data, which was conducted by our team. Here we will share an overview of the network’s performance and reliability as a whole. In terms of individual sensor performance, the participation of 14 different communities offers the opportunity to examine performance with respect to reference instrumentation across different field sites, in different environments. We will also share several examples of the data analysis, which was conducted with the aim of providing insight into communities’ questions regarding sources of interest. This initial analysis has already led to valuable insights regarding the usefulness and limitations of data from low-cost particulate matter sensors, insights that we anticipate will be valuable to other individuals and communities interested in leveraging sensors to learn more about their local air quality.

9AS.21

Inferring Aerosol Types and Sources from Low-Cost Air Quality Sensor Measurements: A Case Study in Cambridge, Massachusetts. AMANDA GAO, David Hagan, Jesse Kroll, MIT

Most studies of low cost sensors (LCS) in urban air quality research have focused on gaining accurate concentration measurements from LCS when compared to reference instruments, enabling accurate estimates of pollution levels and human exposures. While these efforts are extremely useful, it is also desirable to use LCS in other applications that can give valuable insight into air quality--without necessitating the sometimes extensive calibrations required for accurate pollutant concentration measurements. Here, we investigate how LCS can be used to better constrain classes and sources of particulate matter and urban pollutants for air quality and regulatory applications. We present a case study where a multipollutant LCS system, outfitted with low-cost CO, NO₂, O₃, and SO₂ electrochemical sensors and an optical particle counter, was used to collect air quality data at a site in Cambridge, Massachusetts (a relatively unpolluted urban environment) over the course of several weeks. Results from factor analyses (including non-negative matrix factorization) of LCS measurements were then compared to data collected from co-located research-grade particle- and gas-phase instruments. This work provides insight into how multipollutant LCS measurements, despite their inherent limitations, can provide useful information on the sources of particulate matter in an urban environment.

9AS.22

Low-Cost Sensing to Assess Personal Exposure in a Heavily Burdened Air Basin. KHANH DO, Haofei Yu, Cesunica E. Ivey, *University of California, Riverside*

The South Coast Air Basin of California (USA) is well-known for its historically poor air quality. In recent years, the Basin has seen tremendous progress due to the implementation of effective emissions mitigation strategies. The Basin is still subject to poor air quality due to the expansive network of rail and interstate corridors, high volume of shipping activity in the ports of Los Angeles and Long Beach, and operations of several industrial point sources. Further, meteorological conditions in the Basin are conducive to photochemical smog formation due to landward sea breeze, the opposing mountain range, temperature inversions, and infrequent rainfall. The approximately 18 million residents of the South Coast Air Basin are subjected to high levels of primary and secondary particulate and ozone pollution as a result. In this work, we seek to determine the spatiotemporal variability in personal exposure to PM_{2.5} in the inland portion of the Basin, where emissions sources are commonly adjacent to residential areas and secondary pollutant formation is extensive. Further, few personal exposure studies have been conducted for the inland Basin compared to the neighboring, coastal counties of Orange and Los Angeles. In a pilot study, we measure daily PM_{2.5} exposure for 18 community participants from diverse backgrounds each for one week using real-time, wearable monitoring technology that samples every 15 seconds. Participants are also outfitted with fast-response GPS data loggers for precise microenvironment characterization. Results elucidate the microenvironments in the Inland Basin that pose the highest risks for PM_{2.5} exposure. We stratify results using 2010 Census data to investigate the relationship between socioeconomic status and exposure in this unique, mixed land-use area.

9AS.23

From Data Retrieval to Performance Evaluation: PurpleAir Sensor Collocation Across Phoenix, AZ. IAN VONWALD, Karoline Barkjohn, Sue Kimbrough, Ben Davis, Hirna Patel, Ira Domsy, Ron Pope, Andrea Clements, *U.S. EPA Office of Research and Development*

PurpleAir particulate matter (PM) sensors are becoming increasingly popular with non-expert and professional scientists for a variety of applications, such as personal exposure tracking and real-time source identification. However, there is some uncertainty in the data provided by these sensors, as their performance in different and extreme environments has not been thoroughly evaluated. In this study, PurpleAir sensors were studied at 3 regulatory monitoring sites in Phoenix, Arizona to understand the various sensor outputs, evaluate sensor performance, and explore the development of a local correction factor. At each monitoring site, at least 3 PurpleAir sensors were collocated with a Thermo Scientific TEOM between November 2018 and May 2019. A Teledyne T640x was also operated at 2 of the sites. Results including inter- and intra-site comparisons of PurpleAir sensors, comparison of sensors to reference monitors, and evaluation of impacts from extreme environmental conditions (e.g., high temperature and PM, low humidity) on sensor performance and correction will be presented. This work is the first step in a long-term project using PurpleAir sensors to explore the impacts of woodsmoke on particulate matter levels in Phoenix. This investigation will improve our understanding of PurpleAir sensors in new environments, help to streamline future analyses of sensor data by non-expert and professional scientists, and provide the basis for generalizing sensor evaluation and data correction to a national scale.

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9AS.24

Design and Development of a Cylindrical Calibration Chamber for Laboratory Evaluation of Low-cost Particulate Matter Sensors. TOFIGH SAYAHI, Dylan Kaufman, Tom Becnel, Kamaljeet Kaur, Anthony Butterfield, Scott Collingwood, Yue Zhang, Pierre-Emanuel Gaillardon, Kerry Kelly, *University of Utah*

The performance of low-cost PM sensors is commonly characterized using laboratory calibration. This type of calibration typically exposes the sensors and a reference monitor to PM inside a cubic chamber. Few studies have provided an evaluation of the ability of their calibration chamber/procedure to provide a uniform particle distribution. In this study, we designed and evaluated a cost-effective cylindrical calibration chamber capable of continuously providing a uniform PM concentration simultaneously to 8 low-cost PM sensors. The chamber development and evaluation were based on a Computational Fluid Dynamics (CFD) model and a rigorous experimental protocol. Using both of these strategies, we systematically evaluated the ability of the chamber to generate stable PM concentrations and to produce repeatable calibration curves, regardless of sensor position within the chamber. We also used this new chamber to assess 242 Plantower PMS 3003 sensors from two purchased batches. The CFD model and experimental results showed that the chamber is capable of providing a uniform PM concentration to calibrate eight sensors at one time within 6% concentration difference and with excellent reliability (intraclass correlation coefficient > 0.771). We also performed a CFD simulation of a cubic chamber with the same volume and under the same conditions and found a greater concentration difference (16.4%). The results identified two malfunctioning sensors and demonstrated that all the sensors (except for the malfunctioning sensors) were highly correlated with the DustTrak reference monitor ($R^2 > 0.978$). The study also identified significant response differences between batch I and II. As in several other studies, the PMS sensors exhibited a statistically significant difference in their responses to two different aerosol types. Overall, this chamber can be used to complement field observations and help to eventually determine whether good laboratory performance of a low-cost PM sensor indicates its good performance under real-world conditions.

9AS.25

BevoBeacon: A Low-Cost Sensor Platform to Monitor Indoor Environmental Quality. HAGEN FRITZ, William Waites, Sepehr Bastami, Kerry Kinney, Zoltan Nagy, David Schyner, *University of Texas at Austin*

Air quality monitoring is one research area that has taken to using low-cost sensors to determine spatio-temporal concentrations of various pollutants. In this paper, we present the BevoBeacon, a low-cost research platform for environmental monitoring. The BevoBeacon is built around a Raspberry Pi microcomputer extended with custom interface hardware to connect an array of sensors. It gathers temperature, relative humidity, particulate matter (PM) and volatile organic compound concentrations as well as wireless hosts using WiFi and Bluetooth. The software architecture is modular, allowing a BevoBeacon to be augmented with external sensors. Here we describe the sensor apparatus, the validity of the data gathered from the BevoBeacon's PM sensors through comparison to more robust instrumentation in stainless steel environmental chamber, and results garnered through a small pilot study conducted at UT Austin.

The BevoBeacon is housed within a small unit that can be easily transported and installed in any indoor environment. Data is stored locally as well as transmitted for storage in a secure, centralized repository. Initially, the BevoBeacons were placed in a 384 ft³ stainless steel chamber that was seeded with various sizes of Arizona Test Dust. Concentrations and counts measured by the BevoBeacon were compared to those measured by an aerodynamic particle sizer (TSI Instruments, Shoreview MN). To determine the performance of the BevoBeacon in the field, the platform was distributed to 30 students during the academic year and placed in the individual's bedrooms where data were collected for approximately one week.

The BevoBeacon represents an open-source platform that is flexible, available for quick and easy modification, and able to be deployed at scale. The BevoBeacon has the potential to influence future research projects and can be combined with other low-cost sensing technologies to help further the field of indoor environmental quality monitoring.

9AS.26

A Data-driven Approach for Detection of Toxic Metallic Particulate Matters Using Spark Emission Spectroscopy and Machine Learning Algorithms. SEYYED ALI DAVARI, Anthony S. Wexler, *University of California, Davis*

Toxic metal particulate matter (PM) has been associated with serious health issues. Conventional techniques for measuring their atmospheric concentration are limited by cost, cumbersome sample preparation and poor time resolution. Spark emission spectroscopy is introduced as a portable, modular and yet affordable instrument to quantify these compounds in real time. Each analysis results in a high-dimensional spectrum, which can be difficult to interpret specially for poor resolution spectrometers. To detect useful features from the spectrum and improve the detection limits and reliability, an unsupervised learning algorithm was combined with two supervised learning algorithms. Specifically, a K-Means clustering algorithm was employed to address shot-to-shot variations as well as inherent faults due to low-cost components. Then, partial least square (PLS) regression and least absolute shrinkage and selection operator (LASSO) were applied for quantitative predictions. Various hazardous metal elements such as Cr, Pb and Ni were analyzed. The technique provides an affordable, real-time approach compared to conventional techniques such as ICP-OES and XRF.

9AS.27

Utilizing Hygroscopicity of Aerosols to Develop Corrections for Low Cost Air Quality Sensors. SAHIL BHANDARI, Brandon Feenstra, Ashley Collier-Oxandale, Wilton Mui, Vasileios Papapostolou, Andrea Polidori, *South Coast Air Quality Management District*

Low cost sensors (LCS) provide the opportunity for sampling at higher spatiotemporal resolution while minimizing costs. The ability to map the large variability in individual personal exposure makes LCS especially relevant to air quality agencies. However, LCS need to undergo multiple data corrections in an attempt to meet the performance standards of EPA-approved methods instruments. Purple Air PA-II is an optical PM sensor, with thousands of devices deployed across the five continents. The sensor uses proprietary algorithms to convert measured particle counts to particle mass. Recent work on sensor-specific laboratory calibrations did not account for climate-controlled and species dependent hygroscopicity of aerosols.

Theoretical work by Petters and Kreidenweis (2007), validated by laboratory experiments, addresses this issue using a physically meaningful, species-specific, and size-dependent single parameter model that quantifies the hygroscopicity parameter κ for species and their mixtures. Over the period 2016-2018, the Air Quality-Sensor Performance Evaluation Center (AQ-SPEC) at the South Coast Air Quality Management District conducted a long term study to evaluate the performance of PA-II sensor against the FEM GRIMM EDM 180 and 24-hour gravimetric measurements from the EPA Chemical Speciation Network (CSN).

Using results from this field evaluation, we utilize estimated κ from GRIMM to quantify collection efficiency and volume equivalent diameter in each bin measured by the LCS. Here, we compare this effective κ to that obtained from an external mixture assumption of source-apportioned speciated gravimetric mass from CSN. We further compare the size-species resolved κ to size-only estimates and mass-only estimates.

Utilizing these corrections, we can better quantify PM_{2.5} mass measurements based on number counts in LCS with proprietary algorithms. These PM_{2.5} measurements could be used in source apportionment models and their performance quantified relative to measurements from regulatory and research grade instrumentation.

9AS.28

Performance Evaluation of Light Scattering PM_{2.5} Sensors for Deployment in an Urban Sensing Network in Bangalore, India. JONATHAN GINGRICH, Mark Campmier, Advaita Byerreddy, Shayan Charolia, Heather Howton, Brian Mai, Meenakshi Kushwaha, Elbin Savio, Adithi Upadhyaya, Sreekanth Vakacherla, Julian Marshall, Joshua Apte, *University of Texas at Austin*

Low-cost aerosol devices offer the potential to fill critical data gaps on air pollution for cities. Here, we present data on the performance evaluation of 60 PurpleAir (PA) PA-IISD devices in Bangalore, India.

We established an ambient air evaluation site on the ~15m roof of a suburban office building in June-July 2019 with two beta-attenuation monitors (BAM-1022, US EPA FEM designation). Each PA device consists of two Plantower light-scattering sensor modules (PMS5003), resulting in 120 total sensors tested. Colocation of all devices lasted from June 20 to July 8, 2019, resulting in 441 hourly measurements. Hourly BAM PM_{2.5} concentrations averaged 10-40 $\mu\text{g m}^{-3}$.

113 sensor modules were included in the analysis, as seven modules failed during colocation. Sensor-to-sensor comparisons between the PurpleAirs resulted in a high correlation. The hourly median pairwise R² for all combinations of the sensors was 0.99, although 15 modules had median R² values consistently below 0.90. The NRMSE ranged between 0.01 and 0.46 with a median of 0.02. The median pairwise slope was 0.97.

Because BAM measurements are imprecise at their native hourly averaging time, the correlation between the PA sensors and the BAM greatly increased as averaging time increased. For hourly data, there was weak correlation between PA and BAM measurements (median R² = 0.19, median NRMSE = 0.34, median slope = 0.46). For daily averaged data, the relationship improved dramatically (median R² = 0.81, median NRMSE = 0.11, median slope = 0.71). Care must be taken in comparing the PA data to BAM measurements for hourly measurements. At the daily time scale, the PA sensors track BAM readings well and are capable of resolving moderate (~10-20%) concentration differences.

9AS.29

Long-Term Performance Evaluation of the PurpleAir PA-II Sensor in New Delhi, India. MARK CAMPMIER, Shahzad Gani, Joshua Apte, *University of Texas at Austin*

India experiences some of the worst particulate air pollution in the world, with the highest number of deaths from ambient air pollution. Delhi is particularly polluted, experiencing annual mean PM_{2.5} mass concentrations in the range of 120-160 µg/m³. Low cost optical aerosol instruments have attracted attention as a means of augmenting reference methods, especially in environments with comparatively few official monitors. However, many assumptions are made by OPCs when deriving mass concentrations from aerosol light scattering, and therefore in-situ calibration is vital.

From July 2018 through June 2019, two PurpleAir PAII units (each comprising two Plantower PMS5003 sensors) were collocated with a regulatory grade instrument (MetOne BAM-1020) located in the diplomatic quarter in Delhi. Simultaneously, at the IIT Delhi campus, about 5 miles from the site, a Scanning Mobility Particle Sizer (SMPS) and Aerosol Chemical Speciation Monitor (ACSM) were also operated to understand particle size distribution and composition.

Over the course of the entire calibration period, PA attained an OLS R² ranging between 0.65 and 0.70 for the four sensors. The RMSE ranged between 57 – 62 µg/m³ with a NRMSE range of 0.46 to 0.50. After aggregating to 8-hr block averages, R² improved to 0.84 - 0.85, and NRMSE improved to 0.34 – 0.37, with no significant improvement for longer averaging times. After dividing the year of data into seasons, the R² for the Fall period was 0.75, while the monsoon season R² was below 0.3. The most likely cause for this precipitous drop in performance is the influence of water vapor content on mass concentration, and size distribution. Average diurnal profiles showed that while absolute concentrations differed, both PA and the reference instrument captured early morning peaks and afternoon troughs.

9AS.30

New Concept for a Low-Cost Particulate Matter Sensor Based on Rolling Filter Tape Light Attenuation. ELIZABETH CORSON, Jennifer Therkorn, *Johns Hopkins University Applied Physics Laboratory*

Many low-cost optical particle counters (OPCs) are commercially available that count/size particulate matter (PM) in the airstream. These low-cost sensors have limits to the range of particle sizes and concentrations that can be accurately measured, and can be very inaccurate in high humidity. Here, a new concept is proposed for PM measurement that may address these issues; this sampler will collect PM onto a rolling filter tape and read the PM mass loading with a low cost light sensor/LED combination. Integrating PM collection over a short time period (5-min, 1-hr), and then reading the filter, mitigates issues of high concentration and provides near real-time data. A pilot study was conducted to collect total suspended PM in an urban setting across various conditions using a Button Sampler with PTFE filters; this provided a range of loaded PM mass across the filters with four sample filters and one clean blank. A breadboard prototype costing less than \$40 was assembled consisting of a light sensor (high dynamic range digital light sensor, Adafruit), an LED light source (NeoPixel Jewel LED, Adafruit), and an Arduino Uno. To control the distance from the filter and background level of light, the light sensor and LED were positioned across from one another in an assembly to take readings of the amount of light penetration through each filter (lux units). Plotting lux units versus time-weighted PM_{2.5} air quality index as reported from the nearby state air quality monitoring station resulted in a strong linear relationship (R² = 0.89). Overall, this approach appears to be a very promising alternative method to the development of a low cost PM sampler. Future work will include prototype building and model training to calibrate PM mass loading (i.e., mass concentration) with lux unit measurements.

9AS.31

Using Low-cost Sensor Networks to Identify the Influence of Outdoor Air Quality and Indoor Activities on Indoor Air Quality. JIAYU LI, Aliaksei Haurlyiuk, Albert Presto, *Carnegie Mellon University*

Indoor air quality is critical for human health since an average person spend approximately 22 hours, 90% of daily life, inside buildings. Exposure to polluted indoor air may cause fatigue, headache, nasal irritation, and respiratory infections. Indoor air quality is also highly coupled with outdoor air quality, due to the ventilation procedure operated by the heating, ventilation, and air conditioning (HVAC) system. In this study, a network of real-time affordable multipollutant sensors (RAMPs) was deployed at both indoor and outdoor locations in Pittsburgh to investigate the influence of the outdoor air quality and indoor activities on the indoor air quality. The concentrations of ozone and size-resolved particulate matter (PM) concentrations reported by RAMPs will be analyzed. PM can be generated from various indoor and outdoor activities, and the influence of PM on human health has been studied extensively in previous literature. Ozone, as a primary outdoor pollutant generated by transportation and industrial emissions, can be transported into buildings through ventilation. The patterns of indoor air quality changing with outdoor air quality will be demonstrated for polluted and clean days respectively. Furthermore, the contributions of indoor activities (especially occupancy level) to the indoor air quality will be examined. Principle component analysis and a machine learning algorithm will be used to determine and classify primary parameters that influence indoor air quality. When comparing the indoor air quality with outdoor air quality, conventional methods usually focus on one building only. Using low-cost sensors for such comparison can greatly enlarge the dataset by deploying them in multiple buildings, which is beneficial for obtaining more general conclusions, regardless of the differences among buildings.

9BA.2

Size Distributions and Emissions of Fluorescent Biological Aerosol Particles in an Office. TIANREN WU, Brandon E. Boor, *Purdue University*

Human occupants are a major source of bioaerosols in indoor environments. Many processes that influence the emissions and removal of bioaerosols in buildings are dynamic and change over time. Human-driven particle resuspension from flooring, furniture, and clothing is very much linked to human movement and occupancy patterns, which can change throughout the day. The transient operation of HVAC systems affects the delivery of outdoor bioaerosols to indoor spaces and bioaerosol removal via ventilation and filtration. Real-time detection of fluorescent biological aerosol particles (FBAPs) via laser-induced fluorescence (LIF) offers a foundation to probe time-dependent indoor bioaerosol dynamics. The objective of this study is to investigate how occupancy patterns influence the size distributions and emissions of FBAPs in an occupied office.

A four-month measurement campaign was performed from February-May 2019 at the Herrick Living Laboratories at Purdue University, which are four open-plan offices with precisely controlled HVAC systems. Time-resolved size distributions of FBAPs from 0.5 to 20 μm were measured via a LIF-based instrument, the Wideband Integrated Bioaerosol Sensor (WIBS), for one office with hard vinyl flooring and a maximum occupancy of twenty graduate students. The WIBS was enclosed in a fan-cooled soundproof box and sampled indoor air via a vertical copper tube at an inlet height of 1.3 m. Supply air was delivered to the office via an underfloor air distribution system with floor swirl diffusers. Occupancy was monitored via chair-embedded thermocouples and carbon dioxide concentrations. Supplemental measurements of outdoor FBAPs were made via an isokinetic probe directed to the outdoor air duct of the HVAC system.

Size-integrated number concentrations of FBAPs and total particles increased with increasing occupancy in the office. The mean number concentrations of FBAPs and total particles during high occupancy periods (09:00-18:00) on weekdays were 2,700 and 8,000 m^{-3} , respectively, while those during low occupancy periods (18:00-09:00) were 1,000 and 4,700 m^{-3} , respectively. The peak of the mean number size distribution of indoor FBAPs was not fully captured by the WIBS as the modal diameter was $< 0.5 \mu\text{m}$. This peak is likely caused by sub-micron non-biological fluorescent interferences. A sub-mode in the mean number size distribution of indoor FBAPs was observed at $\sim 2.6 \mu\text{m}$, which is likely associated with bacterial cell agglomerates and fungal spores. The ratio of FBAPs to total particles (N_f/N_T) increased with increasing particle size. Size-resolved FBAP emission factors ($\text{no. h}^{-1} \text{ person}^{-1}$) will be determined via integration of a material balance model and time-resolved occupancy data. Hierarchical agglomerative clustering (HAC) analysis will also be conducted to differentiate non-biological fluorescent particles from bioaerosols and to improve the classification of FBAPs.

9BA.3**Summertime Bioaerosol Loadings above the Arctic Ocean.**

ANNE PERRING, James Churnside, Ru-Shan Gao, Richard Marchbanks, Braden Mediavilla, David Fahey, *Colgate University, CIRES CU Boulder*

Large fluorescent bioaerosol (>0.5 μm) was measured over the Arctic Ocean during the summer of 2017 using a Wide-Band Integrated Bioaerosol Sensor (WIBS-4A) installed aboard a NOAA Twin Otter aircraft which was also equipped with an optical particle sensor for in-situ accumulation mode aerosol measurements and a LIDAR for detection of phytoplankton in the water column and aerosol layers below the aircraft. Sampling took place out of Utqiagvik on the North Slope in Alaska, over both the Bering and Chukchi seas, with ice coverage varying from open water to packed, broken ice. Most sampling took place at 1000 feet above the ocean surface with periodic profiling that included legs at 200 feet and 3000 feet. Fluorescent bioaerosol loadings near the ocean surface are analyzed in conjunction with LiDAR-observed underwater phytoplankton layers to assess possible oceanic emission of fluorescent bioaerosol in regions of marine biological activity. Measurements aloft show a large variability in bioaerosol loadings, indicating episodic transport from terrestrial environments and suggesting a strong bioaerosol source from Arctic environments in the summer. These observations can be used to constrain regional bioaerosol sources and to estimate the potential nutrient input to the surface ocean from long-range transport of terrestrial bioaerosol and subsequent deposition.

9BA.4**Impacts of Ambient Bioaerosols to an Unoccupied Indoor Bioaerosols during and after the Hazy Events.** FENG ZHOU, Mutong Niu, Tianle Zhu, Fangxia Shen, *Beihang University*

People spend most of their time indoors. Inhalation of bacterial aerosols is linked to series of adverse health problems, such as rhinitis, asthma and chronic bronchitis. Indoor microbial sources include human, surface dust, ambient atmosphere and so on. As the heavily polluted weather happens frequently in China and other regions, there are a growing body of studies regarding the bioaerosols in the ambient environments. This furtherly raises the health concern of indoor bioaerosols originated from the polluted ambient air. Here we performed a sampling campaign in an indoor environment without occupants, aiming to identify the contribution of outdoor source to indoor airborne bacteria. Air samples were collected from the indoor room and the adjacent outdoor air simultaneously every two hours on both clean and polluted days with a high-flow portable biological aerosol trap (HighBioTrap P-1000). The ACR (air change rate) of the indoor room were measured by using CO₂ as a tracer gas. Levels of total bacteria and viable bacteria were quantified with qPCR (quantitative polymerase chain reaction) and PMA-qPCR, respectively. Meanwhile, the bacterial community structure was identified by a high-throughput sequencing technique.

Preliminary qPCR results showed that the concentrations of outdoor total and viable bacteria were higher than that of the indoor environment. Significant correlation was seen between outdoor total bacteria and indoor total bacteria ($r=0.58923$, $p<0.05$), indicating the contribution of outdoor bacteria to that of the indoor. Nevertheless, the correlation between the indoor and outdoor viable bacteria was not seen. This may be due to that the viability of indoor bacteria is affected by various factors. The concentrations of outdoor viable bacteria were poorly correlated with PM_{2.5}, PM₁₀, but significantly correlated with outdoor gaseous pollutants O₃, SO₂, NO₂ and CO ($p<0.05$). Further analyses are necessary to figure out the contribution of outdoor source to the indoor bioaerosols. These preliminary results also suggest the importance of considering the indoor air pollutants regarding the status of indoor airborne microbes.

9BA.5

Pollen Grains Impacting the Region of Paris: Speciation, Temporal Variations and Geographical Origins. Roland Sarda-Esteve, Dominique Baisnee, JEAN-EUDES PETIT, Valerie Gros, CEA

Pollen grains account for a significant fraction of bioaerosols. Mainly through the inflammation of respiratory tracts, they have a significant health impact, notably in polluted urban areas, characterized by an increase of asthma cases. The understanding of the parameters driving pollen grains concentrations becomes thus essential, especially within a changing climate and increasing urbanization. Multi-year sampling and speciation of bioaerosols have been carried out from 2015 to 2018 in Paris, France, providing unique insights in the most densely inhabited region of France. Strong inter-annual variability was observed, where Betulaceae pollen was found to be the main specie driving this year-to-year variability, especially during spring. Urticaceae was however found to dominate during summer. The investigation of meteorological parameters highlighted that, in addition temperature and precipitation variabilities, wind conditions play a central role regarding the transport of bioaerosols over the Paris region. The geographical origins of pollen grains were therefore investigated with ZeFir, a user-friendly tool for wind and trajectory analysis. Different wind patterns were observed and will be discussed. These pollen episodes are often associated with pollution events, which could increase the allergenic character of smaller particles. Finally, these results will be put in perspective thanks to unique 30-year climatology of pollen grains in Paris.

9BA.6

Design and Evaluation of a New Electrostatic-based Low-cost Biological Sampler. HEMA RAVINDRAN, Kavindra Kumaragama, Shantanu Sur, Suresh Dhaniyala, *Clarkson University*

Bioaerosol collection methods have gained significant interest for a broad range of applications such as healthcare, national defense, bioterrorism, agriculture etc. Bioaerosol collection has largely relied on techniques such as impingement, impaction, and filtration. Here, we explore the use of electrostatic precipitation for bio-particle collection. We designed a small, low-cost, low pressure drop unit for bio-aerosol sampling based on the principle of electrostatic precipitation. The device was designed for efficient collection of biological particles and for ease of subsequent downstream analysis. We designed a low-cost particle charger to improve the collection efficiency of the sampled particles. The performance of the device was tested using *Bacillus thuringiensis var. kurtsaki (Btk)* as the biological test organism and dust as the non-biological test organism. We were able to achieve a collection efficiency >60% for bipolar and unipolar charged particles. The effect of electric field, exposure times, and the corona discharges from the external air ionizer, on the viability of the collected bacterial species was also determined. We will present design details of the sampler and results from our laboratory performance measurements.

9BA.7

Analysis of Airborne Microbiome Using a Portable Bioaerosol Monitoring and Collection Device. KAVINDRA KUMARAGAMA, Hema Ravindran, Shane Rogers, Shantanu Sur, Suresh Dhaniyala, *Clarkson University, Potsdam, NY, USA*

Environmental bioaerosol monitoring by portable, low-cost devices is recently gaining interest in the context of health monitoring and detection of bio-terror threat. To address such need, we have developed a portable, low cost, low power device in conjunction with a local startup. This device, called IoT Real-time Aerosol Concentration sensor and Biological sampler (TRAC- B), is capable of measurement of aerosol concentration and particle capture for offline analysis. TRAC-B uses a low-cost optical sensor for real-time aerosol concentration measurements and an electrostatic precipitator (EP) to collect airborne particles for offline analysis. In this presentation, we will primarily discuss our measurements made with the EP. EP has a low-cost design that allows for 3D printing, has a low-pressure drop allowing for high sample flowrates with a small fan, and the design is optimized for ease of sample extraction. For a preliminary field study, we have deployed several TRAC-B units in different indoor and outdoor locations within Clarkson University. We analyzed the collected samples using different bio-analysis techniques including, culturing, Sanger sequencing, and next generation sequencing to determine the diversity and abundance of the airborne biological particles in various indoor and outdoor environments. We will present our results from this analysis.

9BA.8

Further Investigation and Application of Passive and Low-Energy Bioaerosol Samplers. SYDONIA MANIBUSAN, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

The Rutgers Electrostatic Passive Sampler (REPS) is a passive bioaerosol sampler that captures particles due to electrostatic fields created by permanently polarized polyvinylidene fluoride (PVDF) film. It was shown to perform comparably to active samplers in outdoor environments, with equivalent flow rates of 2.6 L/min and higher for culturable bacteria. However, initial tests found poorer performance indoors. We hypothesized that this difference in sampler performance was due to less vigorous air movement indoors than in the outdoor environment, where stronger air currents bring particles closer to REPS to be captured by passive means. This hypothesis was tested in a residence, where an air circulator fan operating about 2.5 m away from the sampler provided wind speeds of ~0.6 m/s at the sampler's location. In a separate test, REPS was integrated with a low-power pump (REPS-Active) operating at 0.1-0.5 L/min (0.0034-0.017 m/s air velocity through REPS) to further investigate the effect of air movement on particles captured by REPS. Samplers were operated for 24-72 hours. Reference concentrations were provided by a SAS Super 180 (Bioscience International, Rockville, MD). We found that for culturable bacteria, REPS had an equivalent sampling flow rate of ~ 2 L/min with introduced air circulation, while the equivalent flow rates with natural ventilation alone were ~ 1 L/min. Concentrations of culturable bacteria determined by SAS were ~420 CFU/m³, while those determined by the REPS-Active were above 1,500 CFU/m³. The results suggest that for indoor investigations, REPS should be placed near an air mixing source, e.g., a ventilation duct or fan to enhance microorganism capture. In addition, REPS-active shows a great promise as a low-power sampler capable of preserving microorganism culturability over long-term sampling which would allow quantifying long-term bioaerosol exposures. The findings will be verified by experiments in different air environments.

9BA.9

A New Portable High-flow Aerosol-to-Hydrosol Sampler for Rapid Microbial Detection. XINYUE LI, Maosheng Yao, *Peking University*

Bioaerosol has considerable impact in public health safety, ambient air quality and atmospheric chemical processes with its unique biological components and biological activities. The methods of rapid bioaerosol collection and detection is widely required in many sectors. Traditional bioaerosol samplers always have low sampling flow and not portable. It is difficult to recognize the key microbial species and its concentration timely for various microbial exposure scenarios that require rapid response. So our lab group has developed a new portable high-flow Aerosol-to-Hydrosol sampling technology. The sampling flow rate is up to 400 L/min, just weighs about 3.4 kg. Airborne biological particles in the air are separated by the principle of cyclonic inertia and trapped in a disinfected cube with 2 ml DI-water. The sampler has been tested with Aerosolized *Pseudomonas fluorescens* (Gram-negative bacteria), *Bacillus subtilis* (Gram-positive bacteria), and Polystyrene (PS) uniform microspheres under laboratory controlled conditions. The microspheres were sampled to determine their physical collection efficiency, besides indoor and outdoor ambient air have also been sampled for culturing and quantitative polymerase chain reaction (qPCR) to evaluate the microbial collection in the actual environment. The sampler was found to have a cut-off sizes of about 0.58 μm , the physical collection efficiencies for *Bacillus subtilis* (0.86 μm) and *Pseudomonas fluorescens* (0.61 μm) were 86.7% and 74.2%, respectively. The result of culture counting and qPCR test found that the sampler can collect high concentration and biologically active bioaerosol samples in 2 minutes. However, as the sampling time increases, the evaporation loss of the sample liquid and the increase of the concentration of particulate matter in the sample liquid increase the loss of particulate matter, and the sampling efficiency decreases. Compared with the same type of bioaerosol sampler flow, collection efficiency and portability have been significantly improved.

9BA.10

Successful Collection of Viable Vegetative E. coli on Dry Electret Filters. Andrew Page, Zachary Packingham, Michael Hornback, Stephanie Cantrell, DAVID ALBURTY, *InnovaPrep LLC*

Dissolvable gelatin filters and dry electret filters are widely used for collection of bioaerosols, including both bacterial endospores and viable cells. In this study sponsored by NASA, the collection and elution of vegetative *E. coli* on gelatin filters was compared to collection on dry electret filters, for consideration in developing an air sampler for use aboard the International Space Station and potentially other spacecraft. Bioaerosol studies were performed in a 2.8 cubic meter test chamber section within a recirculating loop windtunnel. Surprisingly, viable collection rates were determined to be higher on the dry electret filters (up to 45%) than on the osmoprotective gelatin filters at equivalent face velocities (11%). Data are presented showing efficiencies and concentration factors using varied sampling rates, filter elution volumes, and collection times. Sample concentration using electret filters was higher than on gelatin filters, with higher viability and smaller final sample volumes.

9BA.11

Decay of Single and Clusters of Bacillus Anthracis Sterne Spores Exposed to UV-C and Solar Light. JANA KESAVAN, Daniel Mcgrady, Jerry Cabalo, Aime Goad, *US ARMY CCDC CBC*

It is important to study the fate of bacteria in the environment as intentionally and unintentionally released bacteria can affect the general public, first responders, and soldiers. Bacterial spores are released in the environment as single spores and as various size clusters. Spores intentionally released from commercial sprayers or other devices will result in large particles containing multiple spores which dry down to form spore clusters. In these larger clusters, the outer layers of bacteria may protect organisms in the center from UV exposures. This study was conducted to evaluate whether single spores and clusters are affected differently when they are exposed to UV-C and solar light. Single spores were deposited on to polycarbonate membrane filters using a Sono-Tek aerosol generator and by pipetting solutions onto filters. Bacteria clusters (2.5 and 4 micron) were generated and deposited onto polycarbonate membrane filters using an ink jet aerosol generator. After exposure of the organisms to UV-C or solar light for varying lengths of time, the particles were extracted from filters and cultured. Percent kill was determined by comparing the number of culturable organisms in the exposed samples to the unexposed control samples. The results indicate that the culturable fraction decreased with increased exposure for both UV-C and solar exposure. UV-C exposure results indicate that the 4 micron particles decayed slower compared to the smaller size clusters and single spores as a result of the protection from the outer layers of particles. On the other hand, solar simulator exposure indicates that all three size particles have similar decay curves. These results agree with the mathematical predictions conducted by our collaborators.

9BA.12

Characterisation of a Rotating Drum for Bioaerosol Survival Studies. EMMA KEYSER, Carwyn Davies, Andrew Scott, *Dstl*

The ability to study an aerosol in a suspended state can be beneficial when assessing the viability or variable factors on viability of a bacterial species over an extended period of time. This can be achieved by rotating a drum; rotational forces together with gravitational forces impart a circular path on the small particles within, which allows suspension for many hours.

Rotating drums can vary in size, volume and design and can have adjustable rotation speeds. As a consequence differing rotating drums may require individual experimental parameters, such as the time to 'fill' the drum to a certain concentration, and the time required to attain homogeneity of particles within the drum to achieve effective and reproducible sampling. These parameters can also be influenced and adapted to meet different experimental requirements.

Dstl has previously utilised in-house manufactured rotating drums, recently a new rotating drum was purchased of a different internal design.

A series of experiments were undertaken to provide information of the experimental parameters required for this individual drum and to compare its function to our in-house design.

These experiments were conducted using a 3-jet Collision to aerosolise *Bacillus atrophaeus* to produce dry 1-3 μm particles at varying humidities. The results enable investigations to choose ideal parameters to reliably meet specific experimental requirements, for example to adjust fill times and consequently be aware of how concentrated the bacterial aerosol suspension is immediately after filling. This work has also allowed direct functional comparison to differing drum designs.

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9BA.13

UV Intensity Calculated in Clusters of Spores Held on Surfaces for Models of the Effects of UV on Viability. STEVEN HILL, Dan Mackowski, David Doughty, *CCDC Army Research Laboratory*

Ultraviolet (UV) light can inactivate bacteria and their spores. Bacteria in agglomerate particles can be partially protected from solar UV, an observation that may explain the increased fraction of atmospheric bacteria associated with larger particles near mid-day. There is a need for increased quantitative understanding of the effects of solar UV and germicidal UV on bacteria in the air or on surfaces. Bacterial spores withstand the effects of UV and other environmental hazards better than vegetative cells. We have mathematically modeled bacterial spores as homogeneous spheres, and calculated UV intensities within illuminated individual spheres and clusters of these spheres using the multi-sphere T-matrix (MSTM) method. The simulated cluster can be held within a sphere which encompasses the spheres of the cluster and fills the spaces between them. This encompassing sphere may be given any appropriate complex refractive index. In our previous calculations, the non-rotating clusters, held in fixed position to simulate clusters on a surface, were not in contact with a simulated surface. In nature, contact with a surface is needed to hold the cluster in fixed position. Because actual physical surfaces reflect light, the question of the effects of the surface on the UV intensities within the cluster has not been treated. To address this problem, the MSTM has been extended to calculate UV intensities within clusters on surfaces. The resulting calculations indicate that the effects of the surface on the UV intensity tend to be largest in the spheres closest to the surface, and are especially large in the spheres with most protection from the UV. Also, the effects of the surface are largest for surfaces with higher absorptivity, for the ranges of complex refractive indexes of the spores and surfaces studied here.

9BA.14

Comparison of Aerosol Samplers for Measurement of *Yersinia pestis* in Aerosols. GREGORY WILLIAMS, Stewart Wood, Sierra Gardner, Melissa Krause, Shanna Ratnesar-Shumate, *BNBI / DHS NBACC*

Yersinia pestis, the causative agent of plague, has caused intermittent outbreaks amongst human populations for over a thousand years. One of the most recent outbreaks occurred in Madagascar from August through November 2017, in which a total of 2,348 confirmed cases and 202 deaths were reported. Of these cases, 1,791 were reported as pneumonic plague, a form of the disease that can result from human-to-human respiratory transmission. Currently, few data exist on the risk of aerosol transmission of plague. To begin to examine respiratory transmissibility of plague, an aerosol sampling device that maximizes recovery of viable or culturable *Y. pestis* needs to be identified. The efficiency of a sampler can vary across different microorganisms, potentially introducing a bias that may lead to underestimation of the presence of viable microorganisms in an aerosol. In the present study, the effect of aerodynamic particle size and aerosol sampler type on the sampling efficiency of *Y. pestis* was investigated. The results of this study demonstrated that liquid impingement techniques provide significantly greater recovery of viable/culturable *Y. pestis* relative to gelatin filters and dry cyclone samplers. Thus, liquid impingement would be recommended as the preferred method in future studies examining the potential for respiratory transmission of *Y. pestis* in an aerosol.

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9BA.15

Evaluation of Boron-Metal Fluoride Reactive Materials for Inactivating Viable Aerosolized Spores Simulating Bacillus Anthracis. SERGEY A. GRINSHPUN, Worrawit Nakpan, Michael Yermakov, Reshmi Indugula, Tiina Reponen, Siva Kumar Valluri, Mirko Schoenitz, Edward Dreizin, *University of Cincinnati*

An explosion or fire outbreak in a bio-weapon facility targeted militarily may release highly pathogenic bio-agents. While most of the released microorganisms will likely lose their viability due to heat stress and other factors, a small fraction may survive and – as bioaerosol – be subjected to atmospheric transport, which represents a major regional and global health risk. Some agents such as Bacillus anthracis spores are particularly stress-resistant. Therefore, novel materials, which can serve as reactive additives to an explosive and release combustion products capable of neutralizing the threat are being developed in the frameworks of the Defense Threat Reduction Agency (DTRA) research program. In the past, our team evaluated spore-inactivating materials containing iodine (e.g., Al-I₂, Al-B-I₂, Mg-B-I₂). This effort has recently been expanded to materials containing another halogen, fluorine. In this study, two powdered materials, B-BiF₃ and B-CoF₂, were prepared by arrested reactive milling and combusted in the presence of viable aerosolized spores of Bacillus thuringiensis var kurstaki (Btk), a widely-recognized surrogate of B. anthracis. The inactivation factor was quantified by comparing culture-based counts from the combustion-exposed and non-exposed samples. The tests were conducted under two heat conditions (low weighted average temperature T≈170°C, and moderate T≈260°C) and at different spore exposure time intervals, t (from 100 ms to 1 s). The inactivation factor increased exponentially with t. Both materials were found extremely potent for inactivating the aerosolized Btk spores with B-BiF₃ being of significantly greater efficiency (99.998% of viable spores were inactivated under the moderate heat condition at t = 660 ms). It was concluded that fluorine-containing materials have a great bio-agent defeat potential.

9BA.16

Small Particle Aerosols of Francisella Tularensis; Characterization and Optimization to Support Pivotal Animal Efficacy Studies. Katherine O' Malley, Jennifer Bowling, Eileen Barry, Karsten Hazlett, DOUGLAS REED, *University of Pittsburgh*

Evaluating vaccines and therapeutics for efficacy in animal models under the FDA's Animal Rule requires development of a well-characterized and reproducible method for challenging animals. For bioterrorism threats like *Francisella tularensis* (*Ft*), aerosol dissemination is the likeliest means of a potential attack. We report here our efforts to characterize and optimize *Ft* aerosol performance, as well as improving precision and accuracy in dosing animals with *Ft*. A number of parameters were assessed for their impact on aerosolization of *Ft* including the choice of nebulizer, sampling device, exposure chamber, relative humidity, *Ft* strain selection and media used for propagation, aerosol generation/collection, and quantification. The Aeroneb, a vibrating mesh nebulizer which significantly improves aerosolization of influenza, was no better than the gold-standard 3-jet Collison nebulizer in aerosolizing *Ft*. Selection of impinger and flow rate through the impinger affected determination of aerosol concentration. Further complicating matters, flow cytometric analysis suggested that a large fraction of aerosolized *Ft* was in a 'viable but not culturable' state. Using Brain-Heart Infusion broth and keeping relative humidity >65% provided optimal *Ft* aerosol performance with little variability between individual aerosols on the same day or aerosols across a number of days. Improved accuracy in achieving desired nebulizer concentration greatly improved accuracy in achieving the desired target median inhaled dose, although precision in dosing between individual animals was not improved. Differences in individual animal minute volume during the 10-minute exposure largely account for the remaining variation. Choice of culture broth also affected outcome in vaccine studies; LVS-vaccinated rabbits survived challenge with lower morbidity and mortality if the virulent *Ft* for challenge was grown in MHB as opposed to BHI. This system is sufficiently robust and reproducible to meet the needs for pivotal efficacy studies but further characterization is warranted.

9BA.17

An Improved Method for Quantification of Ebola virus Titers in Dilute Aerosols. MICHAEL SCHUIT, Rebecca Dunning, Jill Taylor, Katie Beck, Denise Freeburger, Paul Dabisch, *BNBI / DHS NBACC*

While human-to-human transmission of Ebola virus is thought to occur primarily through direct contact with bodily fluids of infected patients, short-range aerosol transmission remains a possibility, particularly in health-care settings. Previous studies have demonstrated that the infectious dose of Ebola virus is low when inhaled by nonhuman primates. However, difficulty quantifying low concentrations of infectious Ebola virus in air samples complicates studies assessing the potential public health hazard associated with aerosols containing the virus. In light of this problem, the aim of the present study was to improve sampling and quantification methods for low concentrations of Ebola virus in aerosols. Five low-flow aerosol samplers were assessed for physical and biological sampling efficiencies with aerosols of Ebola virus, with the results demonstrating that gelatin filters were both logistically optimal for work in a biocontainment environment and the most efficient sampling method overall. Additionally, a microtitration assay using a fluorescent reporter cell line was found to have equivalent sensitivity to several other methods for quantifying viral titers. However, this method utilized an automated quantification method, which improved throughput and minimized subjectivity. This assay also enables viral infection to be distinguished from other sources of cellular pathology, and facilitated recovery of gelatin filters in smaller liquid volumes than would otherwise be possible due to assay interference from high gelatin concentrations. This resulted in a more concentrated sample and an increased likelihood of detecting infectious virus in dilute samples. The combined sampling and assay improvements identified in this study resulted in an improvement in sensitivity of approximately ten-fold relative to other published methods for quantifying Ebola virus aerosols, and lowered limits of both quantification and detection. The improved sampling and quantification methods developed in this study will enhance future studies examining the inhalational infectivity of and medical countermeasure efficacy following exposure to low concentrations of Ebola virus in animal models of disease. These methods will also enhance detection or high-confidence non-detection of infectious virus in the air surrounding infected patients and/or animal models, including in exhaled breath, as well as assessment of the environmental fate of the virus in aerosols.

9BA.18

Displacement Ventilation to Prevent Pathogen Spread during Meat Processing. ALEXANDER ZUNIGA, Maria King, *Texas A&M University*

Bacteria have posed a serious problem to the commercial and private food industries for centuries. Only recently have aerosolized bacteria been seen as a large threat to human health and shelf life of food. The beef industry has a particular hard problem in maintaining a clean environment in the slaughterhouses that process the cattle. Shiga toxin producing *E. coli* (STEC) and Salmonella are two severely prominent bacteria that are recognized in pathogenic spread in the meat industry. The study was conducted in a 13,000 sqft fully operational meat packing facility over the period of three years. Using dynamic monitoring devices, the Wetted Walled Cyclones (WWC), air samples were collected at 100 L/min to acquire a representative analysis of a typical full working day meat packing environment. The sampling locations focused on the dehiding area, hot box, tripe room, and fabrication room. The samples were analyzed by microbial plating, whole-cell qPCR and microbiome sequencing. The facility was modeled using a computational fluid dynamics (CFD) program based on the blueprints of the facility's structure as well as of the mechanical design of the heating, ventilation, and air conditioning system. The concentration of airborne Salmonella and STEC has significantly elevated during the summer months. The computational air flow models that were created based on the facility's layout and ventilation design validated with the collected bioaerosol concentrations enabled the visualization of the pathogen movement in meat processing facilities. The new design created for the optimization of the air flow to improve sanitation will be implemented in the facility for validation and further analysis. Based on the customized air flow pattern models and bioaerosol movement older facilities will have a tool to update their HVAC system to reduce pathogenic spread. New facility construction needs to be planned with optimized air flow pattern design.

9BA.20

Methodology to Estimate Performance of Onepass-type Air Sterilization System Using UVC LED in a Chamber for Inactivating Aerosolized Virus. SUNGJAE PARK, Dae Hoon Park, Jungho Hwang, *Yonsei University, Korea*

This study is aimed to evaluate the performance of onepass-type air sterilization system with virus contaminated air in a sealed chamber by using UVC LED and propose a model to estimate real sterilization performance. A model for predicting the chamber sterilization performance was derived from calculation method of filter-based air cleaner performance. Using the data of sterilization performances obtained from the chamber experiment, the correlation work was applied on the above model. According to the experiment, the chamber sterilization performance was 1.81 times higher than expected by onepass-type system's specification. If the germicidal effect only occurs inside the onepass-type system, the chamber sterilization performance should be less than 1x the spec of the onepass-type system due to the flow in the chamber. Therefore, the above result means that viruses passing through the onepass-type system were being further sterilized as they circulate through the chamber from outside the onepass-type system. This considered to be because the virus was physically damaged even if the virus was not completely inactivated in the onepass-type system. The viruses damaged by the UVC were inactivated itself faster than when they were intact in the air. These results can be utilized as an important data for setting the target sterilization performance in UVC sterilization equipment design such as air sterilizer.

9BA.21

Large Enclosure Decontamination of *Coxiella burnetii*. YOUNG CHOI, Michelle Sunderman, Heather Davis, Cassandra O'Connor, William Richter, Mani Muthalagi, Kevin Hommema, *Battelle*

Coxiella burnetii is the causative agent of Q fever and a Risk Group 3 biological agent that requires a high-containment facility to handle or manipulate this obligate intracellular pathogen. *C. burnetii* is regarded as a difficult microorganism to decontaminate and has been shown to be highly infectious and persistent outside of a host. Battelle has developed an efficacious method to decontaminate *C. burnetii* within a large, complex enclosure using hydrogen peroxide vapor (HPV). Battelle has also reliably quantitated *C. burnetii* viability post-decontamination via real-time PCR. The HPV decontamination methods and the quantitative assay for viability were extensively tested in two phases. **Phase I:** Small-scale study with a Class III biosafety cabinet (*i.e.*, glovebox) that used *C. burnetii*-spiked material coupons. **Phase II:** Large-scale study with Battelle's Aerosol Research and Component Assessment (ARCA) Chamber with the same material coupon types. Both phases analyzed samples taken at seven time-points over the course of a 21-day duration due to the bacteria's prolonged culture requirements as well as to collect comprehensive data for decontamination efficacy and challenge the quantitative assay for viability. The results from both phases demonstrated the following: (1) *C. burnetii* was readily recoverable and viable from the control samples after spiking, drying, and weathering for up to 21-days at ambient environmental conditions. (2) Dried *C. burnetii* was highly susceptible to the various HPV parameters tested. (3) Viability of the control samples was readily differentiated from the non-viable decontaminated samples. (4) Decontamination efficacies for each material coupon type were quantitatively calculated via gene copy numbers from the control versus decontaminated samples. This effort showed that *C. burnetii* can be effectively decontaminated with a commercially available sterilant technology in a standard glovebox or in a large, complex enclosure like an ARCA Chamber.

9BA.22

Comparison of Disease Progression in A/J and C57Bl/6 Mice Exposed to Aerosolized *Coxiella burnetii*. CHRISTOPHER JENSEN, Jeanean Ghering, Aysegul Nalca, Sara Ruiz, *USAMRIID*

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 developed clinical signs to include weight loss and temperature changes. Future experimentation will include the development of a non-human primate model in order to examine the full spectrum of disease and complete both a small and NHP model to aid in medical countermeasure screening.

9BA.23

Tracking the Movement of Antibiotic Resistant Genes in Dairy Farms using Computational Fluid Dynamics. HYOUNGMOOK PAK, Maria King, *Texas A&M University*

The increased use of antibiotics in dairy farms is a major cause of the development and dissemination of antibiotic resistance genes (ARGs). The airborne genes can be transported by the wind and be introduced to various bacterial species via horizontal gene transfer. The spread of multidrug resistance in bacteria poses a serious threat to animal and human health. This is especially relevant to open dairy farms where environmental factors play a significant role. This study examines how computational fluid dynamics (CFD) modeling can be used to create the airflow patterns within the dairy farm and identify the movement of ARGs.

In a dairy farm, which had 36 axial fans for evaporative cooling, a Kirby-Bauer test on different bacterial isolates from twenty manure samples collected along the farm revealed that bacteria located under the first row of fans were more resistant to antibiotics, such as ampicillin, cephalothin, and tetracycline, than those in other areas of the farm. At this area, all the manure accumulated when the floor was flooded for cleaning four times a day. Additionally, this area was shaded at the time of sample collection. A three-dimensional computational fluid dynamics (CFD) simulation of air flow patterns revealed that the area with high antibiotic resistance was not disturbed by the fan-generated air movement. High humidity, low sunlight, and low air movement seem to promote the growth and spread of ARGs, which then can be reintroduced into the dairy farm.

Sequencing the bacterial DNA for each isolate will determine which species carry the antimicrobial resistance genes and experimental air velocity measurements will validate the CFD simulation results.

9BA.24**Comparison of Large Particle vs Small Particle Aerosolized Rabbitpox Virus Exposure in New Zealand White Rabbits (*Oryctolagus cuniculus*).** AYSEGUL NALCA, *USAMRIID*

Rabbitpox virus (RPXV) is an orthopoxvirus that causes severe respiratory disease in rabbits when delivered by small particle aerosol in experimental infections. This model represents an important and informative system to evaluate medical countermeasures against orthopoxviruses because it has a disease course similar to monkeypox and smallpox in humans. It is believed that small particle aerosol exposure would be the major route of infection in the event that orthopoxviruses are used as biological weapons or in a terrorist attack. The small particle exposure represents exposure from an artificial source, but fails to capture the inherent aerosol heterodispersity associated with secondary transmission of poxviruses from infected to naïve host. The large particle aerosol route of exposure plays a significant role in secondary transmission and is considered to be an important, if not the major, natural route of transmission for smallpox in humans. Thus, it needs to be determined, if a larger particle aerosol would induce similar disease progression as the small particle aerosol experiment in rabbits. In order to address this question, groups of rabbits were exposed to different doses of aerosolized large and small particle rabbitpox virus. In the large particle groups, all rabbits show various signs of the rabbitpox disease from mild to severe. The small particle groups also showed mild to severe signs of the disease, but with an earlier onset of the disease compare to large particle exposure groups. This study shows that small particle poxviruses, if used as a biological weapon, would have a more rapid disease progression than large particles of the same virus.

9BA.25**Comparison of the Performance of Pneumatic Atomizers for Inhalation Studies with Ebola Virus.** KATIE BECK, Rebecca Dunning, Michael Schuit, Amy Reese, Jill Taylor, John Yeager, Paul Dabisch, *BNBI / DHS NBACC*

The majority of studies assessing the inhalational virulence of Ebola virus have utilized the Collison nebulizer for aerosol generation. While the Collison nebulizer produces respirable aerosols with a mass median aerodynamic diameter in the 1-3 μm range, it also captures and recycles the majority of the output back into the reservoir, resulting in multiple passes of the suspension in the reservoir through the nozzle over the course of an exposure. Other studies have demonstrated that this recirculation can damage the microorganisms present, potentially altering the virulence upon subsequent inhalation. The aim of the present study was to compare the performance of the Collison nebulizer with that of a single-pass air assist nozzle with Ebola virus, and determine whether the single pass nozzle is comparable to the Collison nebulizer. The results demonstrate that the Collison nebulizer and the air assist nozzle produce similar initial particle size distributions when assessed using a phase Doppler particle analyzer. Additionally, the final particle distributions of aerosolized virus, measured using an Aerodynamic Particle Sizer sampling from the breathing zone of an inhalation exposure system, were similar for both generators, with MMADs $< 2 \mu\text{m}$, and GSDs < 2 . Both atomizers also produced similar infectious aerosol concentrations in the inhalation exposure system. The Collison nebulizer did not appear to damage the virus present in the reservoir, as the infectious aerosol concentration measured in serial samples from the inhalation exposure system did not decrease over the 15-minute test. Taken together, these data demonstrate similar performance between the two pneumatic atomizers, and suggest that the single-pass air assist nozzle may be used as an alternative to the Collison nebulizer for inhalation studies with Ebola virus.

9BA.26

Continuous and Efficient Virus Sampling and Enrichment System. HYEONG RAE KIM, Sanggwon An, Jungho Hwang, *Yonsei university*

Against the shortcomings of long-time consuming sampling or incubation of bioaerosols, enrichment technologies have recently been proposed using microfluidic chip. However, microfluidic chip has a limitation for high air sampling flow rate (up to only a few mL/min). Therefore, microfluidic chip is not realizable for air sampler itself in the field requiring high sampling flow rate for the real-time bioaerosols monitoring.

A possible alternative could be to exploit an air sampler, sampling the bioaerosols and simultaneously enriching them in the sampler continuously. However, commercial air samplers are batch-type samplers which cannot continuously deliver the liquid bioaerosols sample to the sensors connected after air sampler for real-time monitoring. Also, air-to-liquid enrichment rate of these samplers for the single bacteria size (0.8 μm) was as low as 600 to 43,000 min^{-1} . So far, there is no system for continuous sampling and enrichment of airborne virus which exist in air at low concentrations.

Herein we report a continuous and efficient bioaerosol sampling and enrichment system which can be utilized not only for airborne bacteria but also virus particles. For these purposes, an air sampler was developed and optimized for efficient bioaerosols sampling. Concanavalin A (Con A) coated magnetic particles (CMPs) were applied for enriching the bioaerosols.

Bioaerosol capturing performance was evaluated using APS and SMPS. Bacteria (*S.aureus*) and influenza A virus (H1N1) capturing efficiency were 80% and 70.3%, respectively with an air flow rate of 10 lpm and an applied voltage of -7 kV. Enrichment capability of our system was evaluated using PCR device. PCR cycle number was advanced as 5.3 after virus enrichment. The highly enriched bioaerosol sample compensates for low collection efficiency of air samplers and can also allow to monitor bioaerosols rapidly by significantly reducing the bioaerosols sampling or culturing time.

9BA.27

Characteristics of Antibiotic-resistance Bacterial Aerosols and the Removal Efficiency of Biofilter during Composting Process. YUNHAO ZHENG, Hongmin Dong, Yu Zhang, *Chinese Academy of Agricultural Sciences*

Antibiotic Resistance Genes (ARGs) recently draw a global attention that pose a threat to worldwide human health. For the benefit of recycling waste and creating a nutrient dense product for land-use, composting has been the main way to treat livestock manure. As a biological process, antibiotic Resistance Genes (ARGs) and antibiotic resistance bacteria (ARB) tend to escape and can become aerosolized during composting, that not only directly affect the health of workers, but also polluting the surrounding environment. However, the existing research on ARGs and ARB found in bioaerosols were mainly on livestock farms, few published papers are available on these emerging contaminants during the composting process. In this study, the distribution characteristics of airborne ARGs and ARB during composting process were studied by site investigation and laboratory studies. At the same time, this study also analyzes the removal efficiency of airborne ARGs of a biofilter system based on composting. The results of the study would help to assess the potential risk of airborne transmission of ARB and ARGs during composting processes, while providing a theoretical basis to emerging contaminant control, reduction of health risks from bioaerosols containing ARGs and ARB, and prediction of potential hazards.

9BA.28

Efficiency Examination of a Pilot Scale Packed-bed Non-thermal Plasma (NTP) Reactor in Inactivating Airborne Viruses Emitted from a Pig Barn on a Michigan Farm. TIAN XIA, Zijie Lin, Eric Lee, Kevin Melotti, Mitchell Rohde, Herek Clack, *University of Michigan*

Airborne transmission of livestock diseases or zoonotic disease greatly threaten global food security, agricultural industry and public health. In pork industry, porcine reproductive and respiratory syndrome (PRRS) is one of the most significant diseases which can be transmitted through air and caused US farmers \$664 million loss annually. Applying HEPA filtration, the traditional bioaerosol control technology, to ventilation air supplied to pig barns involves structural retrofits to buildings that can be costly, in addition to the periodic replacement of used filters. Non-thermal plasmas (NTPs), on the other hand, can inactivate airborne viruses and bacteria with minimal pressure drop. Our previous experiments using a lab-scale packed bed non-thermal plasma reactor demonstrated effective inactivation of bacteriophage MS2 and PRRS virus as a function of applied voltage and power. In the present study, a pilot scale prototype packed-bed NTP reactor was constructed (by Quantum Signal LLC, Saline MI) and installed at one manure pit exhaust of a pig barn on a local Michigan farm, and its PRRS virus inactivation efficiency was tested on-site. Experiments were conducted about seven days after vaccination, when the PRRS virus shedding rate was likely to be the highest. Two impingers and/or two button samplers 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 total viral genome (qPCR). In addition to PRRS virus inactivation, the study also examined the impact of ambient relative humidity on the discharge behavior within the NTP reactor and demonstrated challenges and failures a bioaerosol researcher may encounter when collecting ambient samples on a pig farm.

9BA.29

Design, Fabrication, and Evaluation of Stationary Electrostatic Bioaerosol Sampler (SEBS) with High Concentration Rate. TAEWON HAN, Nirmala Thomas, Sydonia Manibusan, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

We further advanced our liquid-based electrostatic precipitator with the hydrophobic surface for improved bioaerosol sampling performance, including better maintenance of sample viability and culturability during long-term sampling. This stationary electrostatic bioaerosol sampler (SEBS) incorporates a novel wire-to-wire charger and a newly designed removable collector. SEBS deposits airborne microorganisms onto a narrow, removable, stainless steel electrode (3.2 mm×127 mm) coated by a hydrophobic substance (e.g., commercially available water repellent spray) and then the electrode is transferred into the particle removal system, which is fabricated by 3D printing. The removal system allows using 20-40 microliter droplets that result in very high sample concentration rate. SEBS has been developed as a stand-alone, battery-operated and field-deployable bioaerosol sampler with high concentration rate capable of determining long-term exposures to airborne microorganisms.

The latest SEBS version showed an actual collection efficiency of approximately 60-70% when sampling *B. atrophaeus* bacteria and *P. chrysogenum* fungal spores at 20 L/min for as long as 240 min at $\sim 10^3$ - 10^4 /liter microorganism concentrations. The use of collection droplet of 40 microliters resulted in sample concentration rates of up to 3×10^5 /min. In addition, the device produced very low ozone concentrations (<10 ppb). In the next development stage, SEBS will be tested against other bioaerosol samplers capable of long-term collection, e.g., SASS 2400 (Research International, Monroe, WA) when sampling bioaerosols for 240 min or longer in various indoor, occupational, and outdoor environments. The sampler's physical collection efficiency, viability, and culturability of collected microorganisms will be determined using microscopy, adenosine triphosphate (ATP), flow cytometry (Live/Dead test), and culture techniques. The ultimate project goal is to have a reliable bioaerosol sampler capable of long-term particle collection while preserving bioaerosol viability and culturability.

9BA.30

Investigation of Hygroscopic Properties of Giant Cloud-Condensation Nuclei with an Aerosol Optical Trap and Humidified Tandem Differential Mobility Analyzer. BENJAMIN E. SWANSON, Rachel Bramblett, Amanda Frossard, *University of Georgia*

Understanding the links between aerosol particles, clouds, and radiative properties remains a large uncertainty in predicting Earth's changing energy budget. The ability of a particle to act as a cloud condensation nuclei (CCN) is dependent on both its size and composition. Giant CCN may also have an influence on cloud and precipitation microphysics, and the properties controlling their growth are largely unknown. Natural aerosol particles, such as sea salt and pollen and fungal spore particles have also been observed to behave as giant CCN, in addition to CCN at smaller size ranges. Here, we compare the hygroscopic growth and evaporation of aerosol particles generated from fungal spore and pollen fragments to those generated from seawater and model laboratory aerosol particles.

Anemophilous and entomophilous pollen fragments were investigated for chemical and hygroscopic growth differences. We measured the hygroscopic growth of individual, coarse mode aerosol particles using an aerosol optical trap combined with Raman spectroscopy. We compare those measurements to the growth factors of size-resolved, submicron aerosol particles using the Humidified Tandem Differential Mobility Analyzer (HTDMA). Using the two instruments, we can understand the hygroscopic growth of particles from the submicron CCN range into the coarse mode giant CCN sizes. Fragmented pollen exhibits an increase in hygroscopicity and can act as CCN as a result.

9BA.31

Comparison of DNATrax and Bacillus anthracis Surrogate Resuspension from Subway Surfaces. JOHN ARCHER, Adam Hook, Jerome Gilberry, Denise Aslett, Ahmed Abdel-Hady, M. Worth Calfee, Robert Yaga, Donald Bansleben, *US EPA*

Selection of appropriate biological warfare agent surrogates is crucial to understand fate and transport mechanisms of agents in uncontrolled field environments. An inert, sugar-based surrogate for a biological agent developed at Lawrence Livermore National Laboratory, known as DNATrax[®], has previously been used as a surrogate for *Bacillus anthracis* (*Ba*) spores in controlled aerosol releases. These tests were designed to both measure and verify models of contaminant fate and transport following the release. Since the particle size of a DNATrax particle is similar to a single *Ba* spore and other established non-pathogenic biological spore simulants, its behavior in aerosol transport and deposition is also expected to be similar to *Ba*. However, once the aerosol is deposited onto surfaces, it is unknown as to whether DNATrax is a suitable surrogate to study resuspension from surfaces. To investigate this research gap through a Department of Homeland Security (DHS)-funded study, Environmental Protection Agency (EPA) researchers are evaluating resuspension characteristics of DNATrax and an established biological surrogate of *Ba* (*Bacillus thuringiensis* var. *kurstaki* [*Btk*]) from representative porous and non-porous surfaces. *Btk* was selected because it has been demonstrated to be a suitable surrogate in previous EPA resuspension studies. Following particle seeding of surface coupons (stainless steel and concrete) via a dry deposition eductor system, particles are resuspended via forced air in a controlled resuspension wind tunnel (RWT) designed solely for resuspension comparison studies. Once particles are resuspended, they are transported through the tunnel into a settling chamber for full volume particle sampling and real-time particle sizing. Multiple measurements of particle counts, particle size distribution, DNA copies, colony forming units, and particle characterization are made to compare the resuspension (resuspension fraction) of the two particles under varied environmental conditions (30%/80% relative humidity and wind speeds of 5 and 25 meters per second). Results to date have shown that the designed eductor system produces comparable particle size distributions for two surrogates. Results of the resuspension comparison tests will be presented and will guide the selection of biological surrogate agents for future field studies.

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9BA.32

A Microfluidic Inertial Aerosol Sampler for Continuous, Efficient Collection and near Real-Time Detection of Bioaerosols. LEAH CAROL, Andrea Timm, Ronald Jacak, Christopher Stiles, Brian Damit, *Johns Hopkins University Applied Physics Laboratory*

Infectious bioaerosols pose a significant health threat, and as transmission risks are better understood technologies for detection must advance by increasing collection efficiency and limit of detection. Existing aerosol sampling technologies require pre-analysis processing (not real-time) and use large volumes (mL). Among emerging sampling technologies are microfluidic systems, which can continuously operate and combine with approaches for rapid detection, and produce enriched samples due to low liquid-to-aerosol volume ratios ($\leq \mu\text{L}$). Additionally, they offer low production and operating costs. In this study, we describe redesign of the MicroSampler (Choi et al., ACS Sens), a microfluidic inertial aerosol sampler, for the purpose of viral aerosol collection. Two-phase stratified flow (sampling air and collection liquid) and inertial deposition provide efficient aerosol collection. As aerosols traverse the curved region of the sampler, centrifugal and drag forces result in the transfer of aerosols from sampling air to collection liquid. Physical collection efficiency (CE) was determined using salt particles (0.5-2 μm diameter) and an aerodynamic particle sizer, which measured particle concentration upstream and downstream of the sampler. CE for the MicroSampler-based design and two alternative designs were examined. For equivalent air and liquid flow rates, the MicroSampler-based design and alternative designs outperformed the MicroSampler – CE>99% for all particle sizes vs. CE>98% for particles $\geq 2 \mu\text{m}$, respectively. In addition to experiments, modeling of the air-liquid interface was performed using COMSOL Multiphysics package. Initial models provided validation of the conditions required for stability of two-phase flow and the geometry observed at the water interface. Further modeling focused on optimizing device performance. Experimental results indicate the microfluidic sampler provides a cost-effective solution for continuous, efficient aerosol sampling, and, combined with suitable detection reagents, could offer near real-time detection of aerosolized pathogens.

9BA.33

Development of a Bioaerosol Test Platform for the Evaluation of Biothreat Sensor Performance in Identifying Live BSL-3 Threat Agents. JILL TAYLOR, Benjamin Alvarez, Felix Sage, Thomas Pilholski, Elizabeth Corson, Leah Carol, Brian Damit, *Johns Hopkins University Applied Physics Laboratory*

Sensors to detect infectious bioaerosol are continually being developed and improved upon to meet the need for a reliable early-warning of an airborne biological attack. The evaluation of these sensors' performance with various agents requires aerosol test systems that can simulate natural environmental conditions in a controlled biosafety certified laboratory setting. Current Biological Safety Level 3 (BSL-3) test systems vary in many aspects of their design, most notably in how the sensors are integrated into the test airflow. Each technique has weaknesses – direct injection of aerosol into the sensor inlet presents an unrealistic test condition, whereas whole-system and inlet immersion approaches can be burdened by non-homogenous flow velocities and aerosol concentrations at sensor sampling locations.

The Johns Hopkins Applied Physics Laboratory is currently designing and constructing a new BSL-3 test platform housed in a 5' x 25' x 7' Class III biosafety cabinet that will enable closed-circuit wind-tunnel (up to 4 m/s) exposures via inlet immersion of multiple instruments in series, while ensuring that aerosol concentrations and flow profiles are homogeneous at each sensor. Uniquely, the design consists of a configuration of flow straighteners upstream and downstream of sensor inlets. A combination of matrixed velocity measurements, physical sampling of seeded aerosol particles, and potentially particle imaging velocimetry (PIV) will validate the uniformity of aerosol concentration and flow at each sensor location. In addition to this capability, the test platform will have multiple integrated features including systems to control temperature and relative humidity, a static chamber, and a rotating drum for bioaerosol aging experiments. These features will enable studies in sensor test and evaluation, agent fate characterization, and assessment of personal protective equipment. When completed in the summer of 2020, this test platform will offer enhanced capabilities for the study of infectious diseases for both biological defense and public health applications.

9BA.34

Chemical Modification of Ragweed Pollen Allergens via Ambient Air. RACHEL L. DAVEY, Courtney Seffense, Erick Mattson, J. Alex Huffman, *University of Denver*

Reactive nitrogen and oxygen species can interact with proteins and cause post-translational modifications (PTMs). Common PTMs seen include oxidation, hydroxylation, and nitration. Nitrotyrosine (n-Tyr) formed in the body via PTM, for example, is used as a biomarker for inflammation and oxidative stress. Previous work has shown that with even relatively low concentrations of urban pollutant gases NO₂ and O₃, proteins on the surfaces of pollen particles can be nitrated. Related work has shown for an allergenic birch pollen protein (Bet v 1) that nitration promotes an increased allergenic response, but little is known about other atmospherically relevant pollen proteins. Ragweed pollen (*Ambrosia artemisiifolia*) exists in high concentrations across the US and Europe and represents a significant allergen for a considerable fraction of the population. Here we separately exposed samples of two proteins to ambient air during periods of high NO₂ and O₃ to test for nitration. We used bovine serum albumin (BSA) as an inexpensive protein model as well as Amb a 1, the major allergen in ragweed pollen. The extent of nitration was tested using absorption spectroscopy and two immunoassays. Nitration products were detected on both proteins, suggesting the possibility for the hypothesized reactions to be relevant to urban atmospheres. Preliminary results of the pilot study will be presented.

9BA.35

Culturability, Metabolic Activity and Composition of Ambient Bacterial Aerosols in a Surrogate Lung Fluid. FANGXIA SHEN, Mutong Niu, Feng Zhou, Yan Wu, Tianle Zhu, *Beihang University*

Interactions of particulate matter (PM) and respiratory tract play a crucial role in PM-related respiratory diseases. The majority of the work focuses on the oxidative stress induced by reactions between PM-borne redox-active components and lung lining fluid (LLF). The effects of PM-borne biological components are largely unknown. Of all PM-borne biologicals, bacteria, as living microorganisms, are closely related with inflammatory immune responses. However, its inhalation risk is usually determined without considering the respiratory physiological conditions. In this study, a surrogate lung fluid (SLF) with four typical antioxidants was applied to characterize the ambient bacteria, including concentrations of total bacteria/viable bacteria/culturable bacteria, metabolic activity, bacteria-derived endotoxin, as well as the community structure. Comparing to those determined by SLF, we find that use of PBS leads to an underestimation of the bacterial culturability and metabolic activity. No effect was seen regarding the number of total bacteria and viable bacteria (with intact membrane). Population structure change was seen for bacteria cultured from SLF-collected samples, when compared to that from PBS. Spore-forming bacteria, e.g., genus *Bacillus*, were found to be easily recovered with SLF. This implies that use of PBS could underestimate the bacteria inhalation risk, especially those bacterial endospores. Our work highlights the necessity to consider the respiratory airway environment when evaluating microbial inhalation risk.

9CA.1**Experimental Determination of the Relationship between Organic Aerosol Viscosity and Deposition Mode Ice Nucleation at Upper Free Tropospheric Conditions.**

SABIN KASPAROGLU, Russell Perkins, Paul DeMott, Sonia Kreidenweis, Markus Petters, *North Carolina State University*

Atmospheric aerosols can assume amorphous semi-solid or glassy phase states, where particle viscosity exceeds 10^4 Pa s. Particle viscosity varies with temperature and relative humidity. The viscosity of submicrometer particles can be determined by the preparation of dimer particles using the dual tandem DMA technique, followed by identifying the thermodynamic conditions where dimer particles are relaxing into spheres. Amorphous phase state diagrams that delineate glassy, semisolid and liquid states can be constructed from these data. Below -40 °C some glassy organic particles have been proposed to be able to serve as heterogeneous freezing nuclei in the deposition mode. However, measurements of viscosity in the semi-solid/glassy regime at temperatures less than 0 °C in the aerosol phase are limited. Here we present new experiments using the dual tandem DMA technique that extend the measurement range closer toward upper free tropospheric temperatures. From these data, phase state diagrams over the temperature range -60 °C to 40 °C are constructed. These phase state diagrams are juxtaposed with deposition mode ice nucleation data obtained using a continuous flow diffusion chamber (CFDC). Combined these datasets are used to delineate the conditions where the ice nucleation behavior switches from homogeneous freezing nucleation of haze to deposition freezing nucleation on glassy surfaces.

9CA.3**Scaling Laws for Light Absorption Enhancement Due to Nonrefractory Coating of Atmospheric Black Carbon Aerosol.**

RAJAN K. CHAKRABARTY, William Heinson, *Washington University in St. Louis*

Recent field observations have shown atmospheric black carbon (BC) particles to exist in majority populations as internally mixed with non-refractory materials, including sulfate, nitrate, and organic carbon. These materials condense on BC particle surfaces as layers of external coating, which are typically non-absorbing in the visible solar spectrum but acts as “focusing lens” for the incoming light and results in an enhanced mass absorption cross-section (MAC_{BC}) compared to that for an equivalent external mixture. A broad range of enhancement factors for MAC_{BC} ($E-MAC_{BC}$), from 1.05 to 3.5, has been observed during laboratory and field studies. This large spread in $E-MAC_{BC}$ values accompanied by lack of any established scaling relationship makes it a cumbersome and challenging parameter to incorporate in climate models. Toward addressing this knowledge gap, we applied scaling theory to meta-analyzed observational data on BC light absorption in conjunction with numerically-exact electromagnetic calculations of simulated internally-mixed BC particles. Our results show that MAC_{BC} and $E-MAC_{BC}$ evolve with increasing internal mixing ratios in simple power-law exponents of $1/3$ in the shortwave solar wavelengths ($\lambda = 400 - 900$ nm). Remarkably, MAC_{BC} 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 MAC_{BC} . We elucidate the responsible mechanism based on shielding of photons by a sphere’s skin depth and establish a correction factor that scales with a $3/4$ power-law exponent. Violations of these scaling laws are seen to occur only under scenarios where moderate-to-low amount of condensable coating materials are co-emitted with BC (e.g. vehicular emission).

9CA.4**Interpreting Temporal Changes in OMC/OC Ratios - An Alternative to OC-LAC Thermal Evolution Measurements.**

William Malm, BRET SCHICHTEL, Jenny Hand, Anthony Prenni, Colorado State University

The thermal evolution procedure used by most monitoring programs in the United States to determine carbonaceous aerosol concentrations is referred to as the thermal optical reflectance (TOR) method where an aerosol sample that has been collected on a quartz filter is heated and evolved carbon is characterized as either organic (OC) or light absorbing carbon (LAC). Evolved carbon assigned to OC is multiplied by a factor R_{oc} to achieve an estimate of organic mass (OMC). Over the last 10 years, R_{oc} , estimated through multiple linear regression analysis of data collected in the Interagency Monitoring of Protected Visual Environments (IMPROVE) program, has increased at about a rate of 2% per year, reaching values above 2.0 in many regions of the United States. Analysis of evolved carbon concentration temporal trends suggest that TOR analysis inaccurately bifurcates particulate carbon into the OC and LAC fractions with some LAC being inadvertently and wrongly assigned to the OC fraction. The fundamental problem with assigning a LAC-OC split is that there is not an objective definition of the two analytes we claim to be distinguishing between. Without an objective definition of the distinction between LAC and OC, there is no way this distinction can be traced to fundamental principles. There is only the ostensive definition that the desired distinction is just what this [or that] method delivers. Perhaps total carbon and filter absorption measurements are a better alternative to identifying and tracking refractory and absorbing carbon than TOR derived estimations. In theory, both measurements can be calibrated to traceable standards resulting in stable long-term trends that are directly relatable to the relevant aerosols and emissions causing the measured values.

9CA.5**Major Influence of Secondary Organic Aerosols on Black Carbon Absorption Enhancement in the Region of Paris, France.**

Yunjiang Zhang, Olivier Favez, Francesco Canonaco, Grisa Mocnik, Dantong Liu, Tanguy Amodeo, Francois Truong, Andre S.H. Prévôt, Jean Sciare, Valerie Gros, ALEXANDRE ALBINET, INERIS, France

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, it is still needed to improve the understanding of specific underlying mechanisms 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 of both optical and chemical aerosol properties from March 2014 to March 2017 at a suburban background station (SIRTA) in the Paris region (France).

Submicron non-refractory 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-hy 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 ($= \text{babs} / [\text{EC}]$) and expected values for uncoated BC.

Results showed important BrC contribution to the total absorption in the near UV during the winter season, that could be attributed to residential wood burning activities. Even more interestingly, the observed E_{abs} significantly increased with the mass ratio of secondary aerosols to EC, suggesting a strong influence of this secondary components on BC absorption enhancement. This was further associated with the production of highly oxidized secondary organic aerosols (SOA), especially at summertime. These findings infer that considering the yearly cycle of photochemical SOA production should help better assessing seasonal influences of BC global warming. They also suggest that efficient strategies for the reduction of SOA burden in the atmosphere - including abatement of volatile organic compounds emissions - could significantly weaken the BC radiative forcing, at least over the Paris area.

Reference: Zhang et al, Climate and Atmospheric Science, 1(47), 2018.

9CA.6

Optical Absorption Properties of Brown Carbon Aerosols in the Pearl River Delta Region of China. JUN ZHENG, Zhujie Li, Yan Ma, Haobo Tan, *Nanjing University of Information Science & Technology*

We have conducted a set of comprehensive measurements of aerosol compositions and optical properties at a suburban station in Guangzhou, a megacity in the Pearl-River-Delta region of China. Brown carbon (BrC) source origins and radiative forcing effects were investigated. The particle absorption Ångström exponent (AAE) was deduced and utilized to differentiate light absorption by BrC from that by black carbon (BC). The results showed that the average absorption contributions of BrC were $34.1 \pm 8.0\%$ at 370 nm, $23.7 \pm 7.3\%$ at 470 nm, $16.0 \pm 6.7\%$ at 520 nm, $13.0 \pm 5.4\%$ at 590 nm and $8.7 \pm 4.3\%$ at 660 nm. A sensitivity analysis of the evaluation of the absorption Ångström exponent of BC (AAE_{BC}) was conducted based on the Mie theory calculation assuming that the BC-containing aerosol was mixed with the core-shell and external-mixing configurations. We found that variations in the imaginary refractive index (RI) of the BC core can significantly affect the estimation of AAE_{BC} . However, AAE_{BC} was relatively less sensitive to the real RI of the BC core and was least sensitive to the real RI of the non-light-absorbing shell. BrC absorption was closely related to aerosol potassium content, which was most likely associated with straw burning in the region. Diurnal variation in BrC absorption revealed that primary organic aerosols had a larger BrC absorption capacity than SOA. Radiative transfer simulations showed that BrC absorption may cause $2.3 \pm 1.8 \text{ W m}^{-2}$ radiative forcing at the top of the atmosphere and contribute to $15.8 \pm 4.4\%$ of the aerosol warming effect. BrC radiative forcing efficiency in the studied area with reference to certain aerosol SSA and BrC absorption contributions at various wavelengths were systematically evaluated. Evidently, the BrC radiative forcing efficiency was higher at shorter wavelengths.

9CA.7

Detection of Tar Brown Carbon with the Single Particle Soot Photometer (SP2). JOEL CORBIN, Martin Gysel, *National Research Council Canada*

The single-particle soot photometer (SP2) was developed for the measurement of black carbon particles (or refractory black carbon, rBC), and has recently been applied for the detection of iron oxides in dust and industrial emissions. Here, we investigate the application of the SP2 for the detection of “tar balls” or tar brown carbon (tar BrC), which consist of refractory, infrared-light-absorbing carbon. Tar may generate a unique signal in the scattering and incandescent detectors of the single particle soot photometer (SP2), either by evaporating in the laser beam without incandescing (whereas all rBC incandescences) or by displaying a unique scattering-to-incandescence ratio. For the latter diagnostic, it is important to consider that thickly-coated rBC particles may appear to scatter more light due to their volatile coatings.

We explored the above hypotheses using a test data set of tar BrC, representing marine-engine tar. We identified tar particles as displaying both evaporating-but-not-incandescing behaviour and evaporating-and-incandescing behaviour. In the latter case, tar was distinguishable from rBC because its scattering cross-section at incandescence was up to a factor of two greater than that of soot black carbon (soot BC), for similar incandescence intensities. The incandescence signal observed for tar particles may correspond to internally mixed rBC or to the thermal annealing of tar during laser heating; the latter possibility is considered far more likely. There is therefore a potential positive artifact in rBC mass concentrations due to tar incandescence; we found that this artifact is unlikely to substantially bias SP2 measurements of rBC even in tar-dominated samples like ours, where the mass of tar was three-fold greater than that of soot BC. We predict that the more- and less-graphitized tar samples reported in the literature from different sources may show stronger and weaker SP2 responses, respectively.

9CA.8

Chemical and Optical Properties of BC-containing Particles in Urban and Remote Sites of China. XINLEI GE, Junfeng Wang, Yele Sun, Dantong Liu, *Nanjing University of Information Science & Technology*

Refractory black carbon (rBC) aerosol is a very important climate forcer, and its impacts are greatly influenced by the species associated with rBC cores. However, relevant knowledge is lacking due to scarcity of surface observations of BC and its associated coatings. Here we present highly time-resolved measurement results of rBC core and its coating species at a high altitude remote site in central TP (4730 m a.s.l), and in urban Beijing, China, respectively, by using an Aerodyne soot particle aerosol mass spectrometer (SP-AMS), which exclusively measured rBC-containing particles only. Such two cases represent the very clean and highly polluted environments in China. We found that the rBC over TP was overall thickly coated with an average mass ratio of coating to rBC (RBC) of ~ 7.7 , and the coating species were predominantly secondary in nature, mainly produced by photochemical reactions. Interestingly, we found that the thickly coated rBC was less oxygenated than the thinly coated rBC, mainly due to the influence of a transported biomass burning organic aerosol (BBOA). This BBOA was relatively fresh but able to form very thick coating on rBC. On the other hand, rBC-containing particles in urban Beijing were overall associated with thinner coating, and the organic coating had diverse sources including both primary and secondary origins; On average, more polluted rBC-particles appeared to have thicker coating and more secondary species. We also discussed the light absorption enhancement due to the coating under these two cases.

9CA.9

Multi-year Observations of Black Carbon and Brown Carbon in Bogota, Colombia: Relation to Biomass Burning Tracers and Number of Fires in Northern South America. JUAN MANUEL RINCÓN, Amy P. Sullivan, Juan Felipe Mendez, Ricardo Morales Betancourt, *Universidad de los Andes*

Biomass burning pollution sources can produce regional and global impacts on air quality. South America is one of largest contributors to biomass burning emissions (BB) globally. After Amazonia, BB emissions from the grassland plains of Northern South America (NSA), where both wildfires and agricultural burns occur regularly, are the most significant. The BB season in NSA is characterized by a different seasonality compared to that of Amazonia, with numerous fires occurring between January and March. In this work, we report 3 years of continuous equivalent Black Carbon (eBC) and Brown Carbon (BrC) measurements from an Aethalometer AE33-7. This data is used to identify and quantify the contribution of biomass burning from NSA to Bogota, Colombia's. The measurement site is located upwind of Bogota, at a hill-top 500 meters above the plateau where the city is located. Additionally, PM_{2.5} off-line data using a low-vol sampler and 37 mm quartz filters, has been collected during two three-month long field campaigns. The first campaign was carried out from January to March 2018 (high BB emissions in NSA) and the second one between July and August 2018 (low BB emissions in NSA). The filter samples were analyzed in Colorado State University quantifying biomass burning tracers such as Levoglucosan and potassium ion. OC/EC data was also retrieved from the filter samples. MODIS Active Fire Data and HYSPLIT back-trajectories were used to support the identification of potential biomass burning plumes transported to the city during the fires season. We analyzed the relationship between BrC, OC, Potassium ion, and levoglucosan to identify signals of regional transport of BB aerosols. We found a maximum BB contribution of 10% to light-absorbing aerosols during the high number of fires season and a 1% BB contribution during the low number of fires season. Our results indicate potential biomass burning transport events from wildfires were observed during the months of January and April. In addition, we identified potential source regions, most of them located in the Orinoco basin, as most of the fires were found in this region.

9CA.11

Estimating Volatility Distributions of Primary Organic Aerosols Using Artifact-Corrected Quartz Filters. Alexandra Ng, Hanyang Li, ANDREW MAY, *The Ohio State University*

Recent studies have estimated volatility distributions to represent primary organic aerosol (POA) of some combustion sources (on-road vehicles, open biomass burning), and these volatility distributions have been implemented into chemical transport models for the simulation of regional air quality. However, the derivation of these distributions based on empirical observations may be challenging for other sources. For example, some of the previous work utilized sampling and analytical techniques that may be less readily available, including a thermodenuder/aerosol mass spectrometer system, thermal desorption-gas chromatography-mass spectrometry, and/or complex kinetic models of the observed aerosols. In this study, we investigate the feasibility of estimating volatility distributions from these sources using bare quartz and quartz-behind-Teflon (QBT) filters analyzed by a thermal-optical technique; the combination of bare quartz and QBT enables the correction of the filters for positive sampling artifacts.

We include both open biomass burning samples collected at the Fire Sciences Laboratory in Missoula, MT and light-duty gasoline vehicle (LDGV) samples collected at the Haagen-Smit Laboratory in El Monte, CA. Assuming both gas/particle equilibrium and sample-air-stream/filter equilibrium, we apply the equilibrium volatility basis set approach to derive volatility distributions for both sources. We observe some discrepancies with the biomass burning samples (likely because those experiments were not designed to study organic carbon), specifically under more dilute conditions. However, applying this approach to the LDGV samples results in good agreement with published results. This finding has important implications for the derivation of volatility distributions for other POA sources (e.g., cooking) that are currently unrepresented in the transport models, given that the collection and analysis of quartz filters for organic carbon is something of a standard practice for most source testing.

9CA.12

The Influence of Calibration Standards on the Measurement of the Mass Absorption Coefficient of Black Carbon. ELIZABETH WIGGINS, Richard Moore, Luke Ziemba, Gregory Schuster, *NASA*

Black carbon aerosol (BC) emitted from fossil fuel combustion and biomass burning absorbs incoming solar radiation and influences the physical and chemical properties of the atmosphere. The climate forcing of BC is a highly uncertain and critical parameter in the radiation balance of the planet. Light absorption by BC per mass, the mass absorption coefficient (MAC), is a value widely used by the scientific community to quantify the influence of BC light absorption on the atmosphere and climate. Considerable disagreement exists between past and present laboratory and field-based measurements of the MAC of uncoated BC particles. These disagreements could be an artifact of changing instrumental calibration standards or measurement techniques. For example, a single particle soot photometer (SP2) is often used to measure BC mass through laser induced incandescence. However, the SP2 has to be calibrated using a BC standard with a known effective density. The community recently shifted from using Aquadag as a calibration standard to using fullerene soot, and there has been a corresponding shift in measurements of BC MACs that rely on SP2 derived mass measurements. In this study we measured the MAC of commonly used calibration standards, including fullerene soot, Aquadag (Classic and Lot 9267), and carbon black (Cab-o-jet 200). Our experimental setup included a centrifugal particle mass analyzer (CPMA) to measure mass, a scanning mobility particle sizer (SMPS) to measure size, a single particle soot photometer (SP2) to determine the relationship between BC incandescence and mass, and a differential photoacoustic absorption spectrometer (DPAS) to measure absorption. The results from this study will improve our understanding of the true MAC of BC and highlight the cause of discrepancies between measurement techniques while offering correction factors for previous studies.

9CA.13

Portable Real-time Black Carbon Monitoring Using the MA300: Performance Characterization in Laboratory and Real-world Environments. MRINMOY CHAKRABORTY, Jeff Meiklejohn, Keyhan Babae, Steven Rogak, Naomi Zimmerman, *University of British Columbia*

Black carbon (BC), a powerful climate forcing agent and primary aerosol particle emitted from incomplete combustion, is an important pollutant to consider in air pollution studies, particularly in under-characterized environments (e.g., indoors in rural India). Aethalometers, which use an optical attenuation method, are a popular instrument for measuring real-time BC mass concentrations, but are bulky and difficult to deploy in microenvironments where power and space are limited. The recently developed microAeth MA300 (AethLabs), a portable aethalometer, seeks to overcome these power and space limitations. It is capable of 5-wavelength measurements in both single and dual spot mode and is light, portable, and battery-powered. However, the MA300 is a relatively new instrument, and its performance in different environments (soot generator, urban ambient, wildfire smoke-affected urban ambient) requires assessment.

This study evaluates the performance of MA300 compared to a low-cost BC sensor (ABCD), a 7-wavelength aethalometer (AE33, Magee Scientific) and a DustTrak (TSI) in three different environments: (1) laboratory generated soot particles from inverted burner, (2) ambient measurements at a traffic intersection and (3) ambient measurements during wildfire smoke-impacted periods. The inverted burner provided a stable soot concentration and has been used to examine filter loading corrections. Preliminary comparisons from the inverted burner experiments suggest that without correction, the MA300 tended to overestimate BC concentrations. Ongoing work in ambient environments is being conducted to finalize any MA300 corrections required during different source-dominated (traffic, wildfire) periods.

9CA.15

Numerical Evidence of Blocking Effect of Brown Coatings on the Light Absorption of Internally Mixed Black Carbon. Jie Luo, Yongming Zhang, QIXING ZHANG, *University of Science and Technology of China*

Using the numerically exact multiple sphere T-matrix (MSTM) method, we explored the effects of brown coatings on absorption enhancement (Eabs) of black carbon (BC) at different wavelengths (λ). The ratio of the absorption of BC coated by brown carbon (BrC) to an external mixture of BrC and BC (Eabs_{internal}) is also investigated. Eabs increases with the absorption of coatings, while an opposite trend is observed for Eabs_{internal}. A much wider range of Eabs is observed for BC with brown coatings compared to that with non-absorbing coatings. As the mass ratio of BrC to BC (MR) is over 13.9, Eabs can exceed 5.4 for BC with brown coatings at $\lambda = 0.35 \mu\text{m}$ under a typical size distribution. Specifically, as MR increases to approximately 13.9, Eabs values of larger than 3.96 can be observed at $0.532 \mu\text{m}$, which is a little higher than the commonly measured Eabs of 1.05–3.5 at this wavelength.

Previous studies have focused on the lensing effects of coatings but neglected the blocking effects of absorbing coatings. Eabs_{internal} can be below 1 at an ultraviolet spectral region for BC with brown coatings, which indicates that the absorption of internally mixed BC is less than that of an external mixture of BrC and BC due to the blocking effects of outer coatings, and we named the blocking effect of absorbing coatings the “sunglasses effect”. The lensing effect and the sunglasses effect are clearly defined. Moreover, the effects of composition ratios and the size distribution are explored at different wavelengths. Our findings can improve the understanding of the absorption enhancement of BC with brown coatings.

9CA.16

Characteristics of Organic Compounds in PM_{2.5} Aerosols in Seoul, Korea. SOYOUNG JUNG, Hyewon Kim, Mi Rae Lee, Min Hye Kim, Youngkwon Kim, Jieun Park, Seung-Muk Yi, *Seoul National University, Seoul, Korea*

Fine particulate matter (PM_{2.5}) which is one of the major air pollutants, is emitted by diverse anthropogenic and natural sources and impacts on climate change directly or indirectly. Furthermore, PM_{2.5} is classified as carcinogenic to humans (IARC Group 1) and is able to trigger adverse health effects on cardiovascular, respiratory, and central nervous systems. PM_{2.5} is composed of varied constituents such as water-soluble ions, heavy metals, elemental carbon, and organic carbon. Organic carbon contains various organic compounds which have different emission characteristics depend on each emission source. Thus, identifying the emission characteristic is possible by characterizing the concentration of organic compounds. The aim of this study is to analyze property of PM_{2.5} and to characterize the concentration of organic compounds in PM_{2.5} collected from June 2018 to May 2019 in Seoul, Korea by using the sonication extraction method. The sampling site is located on the rooftop of Graduate School of Public Health in Seoul National University (37.465°N, 126.955°E) in Seoul, Korea. The site is in the southwest side of Seoul and is well known for one of the worst air quality region in Seoul. For the analysis of organic compounds, PM_{2.5} samples were collected using the high volume air sampler (TE-HVPLUS, TISCH, USA). Before the sampling, quartz filters (QMA 1851-865, 203mmx254mm, Whatman, UK) were baked at 450°C for 12 hours to remove pre-existing organic matters. The pre-baked filter was loaded on the sampler with impactor filter (TE-230-QZ, TISCH, USA) to collect particulate matters less than 2.5µm. For sample extraction, quartz filters collected PM_{2.5} sample is extracted by using sonication method. In the sonication method, samples were extracted with 30 mL mixture of dichloromethane and methanol (3:1, v/v) for 30 minutes. This procedure was repeated once more. The extracts were concentrated to 1mL by using nitrogen gas using TurbovapII (Caliper Life Sciences, USA). Final concentrates were analyzed by gas chromatography/mass spectrometry (GC/MS) (7890A/5975C, Agilent Technologies, USA).

9CA.17

Comparing the RDG-FA and T-matrix Methods for Soot Given Information about Polydispersity and Effective Density. Keyhan Babae, Timothy Sipkens, STEVEN ROGAK, *University of British Columbia*

This compares the optical properties of soot aggregates for non-premixed flames, calculated using Rayleigh-Debye-Gans approximation for fractal-like aggregates (RDG-FA) and the multiple-sphere T-matrix method. The techniques are evaluated, considering that the primary particle size and effective density are correlated with the aggregate mobility diameter. The distribution of primary particle size is characterized using a geometric standard deviation, which is a function of the aggregate mobility diameter. Primary particle size is assumed to be constant within each aggregate. For RDG-FA, we use the implementation described in Babae et al. (2019); while, for the T-matrix method, the absorption and scattering cross-sections are interpolated from the database developed by Liu et al. (2019). As a case study, the current work selects a refractive index of 1.6+0.6j, 1.95+0.79j, and 2.0+1.0j at wavelengths of 532 nm, 550 nm, 870 nm, respectively. The work proceeds with a parametric study to determine the sensitivity of the optical properties of the aggregate to the mass-mobility exponent, effective density, and parameters of the primary particle size distribution.

9CM.1

Characterizing Amine Aerosol Emissions from Water-Lean Solvent CO₂ Capture Process. Paul Mobley, Jak Tanthana, Ryan Chartier, David Barbee, Roger Pope, Shaojun Zhou, JONATHAN THORNBURG, *RTI International*

Aqueous (water-rich) amine-based solvents for post-combustion CO₂ capture are the most mature technologies to combat climate change by reducing the CO₂ emissions from large static point sources such as coal-fired power plants. While significant research, characterizations, and countermeasures to suppress amine aerosol emissions associated with aqueous solvents have been developed in the past decade, the same information does not exist for the novel water-lean solvent (WLS) class. Here, our goal is to characterize the aerosol emissions, derive an empirical emissions model, and minimize the overall amine emissions from RTI's eCO₂Sol as well as other WLSs via process improvements and utilization of available emission control technologies. Previous studies found up to 70% of the amine emissions during the CO₂ capture process occur in the aerosol phase. Studies have reported 10⁷ particles/cm³ with CMDs from 10 to 500 nm, are typical aerosol counts and size distributions observed at the vent stack from the aqueous amine solvents.

RTI's bench-scale gas absorption system (BsGAS) evaluated the impact of various operating parameters on amine emissions from the CO₂ capture process using WLS. A simulated power plant flue gas with 13% CO₂, 6% H₂O, and balanced with air at 100 to 300 slpm can be generated at the flue gas generator section. A SO₃ generator introduces 0 to 6 ppm SO₃ into the feed gas stream to create sulfuric acid condensation nuclei. TSI SMPS and APS instruments measure aerosol growth and emissions at the inlet of the CO₂ absorber and outlet of the water wash column. Baseline testing with the SO₃ generator produced total aerosol concentrations in excess of 10⁷ particles/cm³ and large sub-micron aerosol peaks with mean diameters ranging from approximately 30-60nm. The total aerosol concentration and size distribution are correlated to the SO₃ concentration.

9CM.2

Effects of Defects on Adsorption Characteristics of Magnesium Oxide Nanoparticles Synthesized through Aerosol Processes to Gas Air Pollutants. KYUNGIL CHO, Changhyuk Kim, *Pusan National University*

Gaseous air pollutants in flue gas such as sulfur oxide (SO_x), nitrogen oxides (NO_x) and carbon dioxide (CO₂) are regulated because of their adverse effects on the human health and environment. One of the technologies to reduce these contaminants is adsorption and magnesium oxide (MgO) has been investigated intensively as a gas adsorbent. In addition, MgO nanoparticles through aerosol processes can enhance the adsorption efficiency due to the large surface area. In this case, MgO nanoparticles also have intrinsic defects caused by rapid reactions in the air, which have been reported to change optical characteristics of the nanoparticles before. However, the effects of the defects on the adsorption characteristics so far have not been known well. Therefore, the objective of this research was to investigate the effects of the defects of MgO nanoparticles synthesized by aerosol processes on the adsorption characteristics to the gaseous air pollutants. The morphology and crystallinity of MgO nanoparticles synthesized through the self-combustion were analyzed by the scanning electron microscopy and X-ray diffraction, which showed cubic shaped pure crystalline MgO nanoparticles, compared to irregular shapes of commercial one (Sigma-Aldrich Co.). For the adsorption experiment, both self-combustion and commercial MgO nanoparticles were placed in a reaction chamber, and then the chamber was purged with target gases (100% CO₂, 10ppm SO_x or NO_x mixed nitrogen) at 1 atm and room-temperature. After adsorption process, quantitative analysis of Thermogravimetric Analysis (TGA) and Gas Chromatography (GC) were conducted to determine the amount of target air pollutants adsorbed on the nanoparticles. Temperature range for the TGA method was between 25 and 800 °C, and an acid treatment was applied for the GC analysis. Adsorption performances of the two pure MgO nanoparticles are presented, and the effect of defects on the adsorption characteristics will be also discussed.

9CM.3**Simulation of Electrohydrodynamic Flow and Particle Motion in Electrostatic Precipitators Under Turbulent Conditions.**

AUSTIN ANDREWS, Christopher Hogan Jr., *University of Minnesota*

Electrostatic precipitators (ESPs) continue to be a widely applied technology for the collection of particles in coal combustors and electrostatic air cleaners. ESPs are typically operated under turbulent flow conditions, yet the electrostatic body force term can have a non-negligible influence on the fluid flow within ESPs. These collective effects complicate prediction of particle charging, motion, and collection in ESPs from engineering first principles. To better facilitate ESP modeling, we have developed a solver using the open source CFD library OpenFOAM, in which Menter's shear stress turbulence model (RANS) is used with an electrostatic body force term to solve for fluid momentum, ion and particle concentrations are modeled using convection-reaction mass transfer equations (with particles of different size and charge state modeled as distinct species), and the Poisson equation is used for the electrostatic potential. To solve these coupled equations, a custom solver was developed which utilizes a finite volume method with first order solution schemes. The model is validated by comparing the velocity profile in the streamwise (flow) direction in a wire-plate ESP to previously published PIV measurements wherein the electrostatic body force had an appreciable influence on the fluid flow profile. We propose that this solver can be employed to examine particle dynamics in a variety of environments where both turbulent flow and electrostatics are significant.

9CM.5**A Numerical Study for Pressure Drop Across a Two-Stage HEPA Filter.**

Wonyoung Jeon, Byong Hyeok Lee, Jong Cheol kim, Sanghyeon Kang, Hyunjun Yun, YOUNGJIN SEO, *Kumoh National Institute of Technology*

High-efficiency particulate air (HEPA) filters are used in many fields such as medical, industrial, and military. The filter is the form of a pleated filter by densely bending the flat media rather than that of the form of flat media. It is used as a single stage. In this study, a numerical method is employed to predict the pressure drop through the filter in many different conditions. The ultimate purpose of this study is to predict the pressure drop of the two-stage HEPA filter. The size of HEPA filter is 361*277*25 (L*W*H) mm and its pleat pitch is 3.8 mm. The glades of the filter used in the study are H10, H11, H12, and H13. The facial velocities are 0.5, 0.75, and 1 m/s. The resistances of the filter in each condition are predicted and then pressure differentials across the filter in the conditions are numerically calculated. Characterization of the two-stage HEPA filter is being conducted and the results will be reported during presentation.

9CM.6

Application of the Mobile Aerosol Lung Deposition Apparatus (MALDA) on Estimation of Ultrafine Welding Fume Respiratory Deposition. Yi Chen, WEI-CHUNG SU, Macrio Bezerra, Jun Wang, *University of Texas Health Science Center at Houston*

In this study, a mobile aerosol lung deposition apparatus (MALDA) that utilized a set of physiologically representative human airway replicas with different numbers of airway generations was developed. Laboratory evaluation tests were conducted using ultrafine welding fume particles. The ultrafine welding fume particles were generated in a welding fume chamber and delivered to the MALDA for respiratory deposition experiments. A differential method was adopted to calculate the deposition of ultrafine welding fumes in the human tracheobronchial airways. The estimation of the respiratory deposition was facilitated by an empirical model developed according to the experimental data acquired. The estimated cumulative respiratory deposition ranged from approximately 9% to 31% for ultrafine welding fume particles between 10 nm and 100 nm in diameter. This finding indicates the feasibility and suitability of applying MALDA as a useful tool for on-site workplace respiratory deposition measurement for other workplace ultrafine particles.

9CM.7

In Situ Time- and Size-Resolved Particle Removal Efficiency of a HVAC Filter Bank in an Office Building. JINGLIN JIANG, Tianren Wu, Brandon E. Boor, *Purdue University*

The size-resolved removal efficiency of HVAC filters is dynamic rather than static. Many factors can drive time-dependent changes in the *in situ* removal efficiencies of HVAC filters, including the operational characteristics of the HVAC system, relative humidity, deposited mass loading on the filter, and physiochemical properties of the particles to which the filter is exposed. The objective of this study is to evaluate the *in situ* time- and size-resolved particle removal efficiency of a HVAC filter bank in an office building under variable HVAC operational conditions.

A six-month measurement campaign was performed at the Herrick Living Laboratories at Purdue University, which are four open-plan offices with precisely controlled HVAC systems. The HVAC system included a filter bank (W : 36 in, H : 24 in) with a MERV 7 pre-filter (D : 2 in) with synthetic media and a MERV 14 filter (D : 12 in) with layered meltblown synthetic media. Particle size distributions from 6 to 10,000 nm were measured upstream and downstream of the HVAC filter bank with a High Resolution Electrical Low Pressure Impactor (HR-ELPI+) with sintered collection plates. An automated three-way valve sampled particles across the HVAC filter bank at four-minute intervals, switching between two-minutes upstream and two-minutes downstream. More than ten ventilation modes were implemented with variable supply volumetric airflow rates (1000 to 2000 cfm) and outdoor to recirculation air (O/R) ratios (0 to 1).

The *in situ* size-resolved removal efficiency of the MERV 7/14 filter bank exhibited a diel trend due to transient variations in the concentrations and size distributions of the mixed outdoor and recirculation air. The size-integrated particle number (6 to 1,000 nm) removal efficiency was typically greater from 08:00 to 17:00 compared to the evening. This is likely because the upstream particle size distributions were dominated by nucleation (< 10 nm) and Aitken (10 to 100 nm) mode particles during the day and shifted to larger particles during the evening. The median size-integrated particle number removal efficiency increased with increasing O/R ratios from 45% at a O/R of 0, to 49% at a O/R of 0.25, to 56% at a O/R of 0.45, and to 59% at a O/R of 1. Conversely, the size-integrated particle mass (6 to 1,000 nm) removal efficiency decreased from 92% to 71% as the O/R ratio increased from 0 to 1.

9CM.8

3-D Simulation of Submicron Particle Filtration on an Elliptical Fibrous Surface. MING DONG, Jinyang Li, Sufen Li, Yan Shang, *Dalian University of Technology*

Fine particles, as one of the most significant environmental pollution problems, are generally released into the atmosphere from coal-fired power plants, engines, biomass-fired boilers, and so on. Fibrous filters have been widely used to remove aerosol particles from carrier gases due to its simplicity, convenience and high collection efficiency. In this work, a numerical research on the deposition behaviour of submicron particle on an elliptical fibrous surface has been carried out using the CFD-DEM coupled with in-house subroutines. We use a particle interaction model to simulate the particle deposition behaviour on the surface of an elliptical fiber. The model well predicts the formation of the dendrites and the dynamic progression of the deposition. Firstly, for the elliptical fiber, the different angles of orientation relative to the incoming flow increases have little influence on the smaller particle diameter ($d_p=0.5\mu$) due to the dominant diffusion mechanism. It is more obvious on larger particle diameter ($d_p=0.8\mu\text{m}$). Secondly, as the inlet fluid velocity increases from 0.1 to 0.8 m/s, the deposition pattern changes from uniform distribution to branched dendrites. The collection efficiency gradually decreases with increasing inlet fluid velocity. The minimum collection efficiency is occurred at $v_{in}=0.8\text{m/s}$. Thirdly, as particle diameter increases from 0.5 to $1.0\mu\text{m}$, the deposition dendrites significantly change due to different particle capture mechanisms. The collection efficiency increases with increasing particle diameter. The maximum collection efficiency is occurred at $d_p=1.0\mu\text{m}$. Finally, as the solid volume fraction (SVF) of filter increases from 2.8% to 8.2%, the collection efficiency and the normalized pressure drop increase gradually with the increasing SVF.

9CM.10

Charge Characterization of Nanoparticles Exiting Non-thermal Atmospheric Pressure Plasmas. GIRISH SHARMA, Nabel Abuyazid, Sukrant Dhawan, R. Mohan Sankaran, Pratim Biswas, *Washington University in St Louis*

Electrostatic precipitators (ESPs) have been widely employed in coal power plants for particle removal. Traditional ESPs use a corona discharge for particle charging, which are then captured with the DC electric field. Corona is a form of gas discharge with typical values of ion concentration on the order of $10^{14}\text{-}10^{16}\text{ #/m}^3$, which is on the lower end of among atmospheric discharges. Radio-frequency (RF) and kHz driven dielectric barrier discharges (DBD) are observed to be several orders of magnitude larger in ion concentration. Our understanding is that particle charging improves with larger ion concentrations. Thus, we explore the possibility of using RF/kHz plasma for particle capture technologies.

In this poster, we present the charge characterization of atmospheric pressure non-thermal RF plasma and DBDs. First, ion concentration is calculated in the pristine plasma for both plasma power sources, obtained from the resistivity of the discharge. Following this, particle-plasma interaction is studied in two different flow configurations. the first configuration conducts particles through the plasma. In the second configuration, the aerosol flow passes perpendicularly through the plasma region past the ground electrode, so called plasma jet. The plasma jet region is characterized by the relaxation of energetic species, visible from the decay of optical emission. In this region, charged species are still present but to a lesser extent. Despite the decrease in charged species concentration, it still presents promise as the cross-flow configuration introduces flexibility and variety to the charging system.

The particle size distribution, and particle charge distribution is measured downstream of the charged region. Moreover, the fraction of multiple charged particles is measured for the particle size distribution using a tandem DMA system. The performance of AC-driven plasmas is evaluated against the traditional DC corona by comparison of particle charge fractions.

9CM.11**Modeling the Impact of Ventilation Control Strategies on Airborne Infectious Disease Transmission in Schools.**

SANGEETHA KUMAR, Atila Novoselac, Richard Corsi, *The University of Texas at Austin*

This study provides a detailed methodology for assessing the impact of ventilation control strategies on airborne infectious disease, specifically influenza, in schools. A school's indoor environmental quality is known to have an effect on student performance, productivity, and health. Public school systems can incur losses due to sickness-related missed school days. Given the growing evidence that airborne transmission is of importance to influenza, increased ventilation control strategies can be employed to reduce flu-like illnesses. A simulation framework was developed to assess the costs and benefits of airborne disease infection and ventilation energy usage in schools using CO₂ as a measure of ventilation and exposure. The probability of influenza infection in a classroom was approximated by using data from a field campaign in Central Texas schools, reported epidemiological data, and a model developed by Rudnick and Milton (2003). The model is highly dependent on the quanta generation rate or the generation rate of airborne infectious doses of influenza. A fractional removal term was developed to correct for filtration and depositional losses of the infectious quanta generated by the infector. Ventilation energy requirements and associated outdoor air conditioning were estimated using air exchange rates and environmental quality conditions indoors (from the field study) and outdoors. To assess the variability in input parameters, Monte Carlo simulations were performed for varying control strategies, mechanical system types, and fractional removal terms for the peak flu season of December to February. Given the relatively low cost of energy for Central Texas, a hot and humid climate, mild to moderate increases in ventilation rates may prove beneficial for the well-being of students and staff. School systems may strongly benefit from this analysis to make better decisions on ventilating classrooms to reduce financial losses due to sickness related absences during the flu season.

9CM.12**Dioxin Emission Reduction of Medical Waste Incinerators Using Low Temperature Plasma Integration Technology.**

ZHENYU DU, Ting Zhang, Aimin Liu, Zhiguang Zhou, Yixiang Zhang, Rui Zhou, Yue Yu, *CNEAC, China*

Low temperature plasma integration technology could destruct macromolecules and converse their valence state, and thusly has an advantage on dioxins reduction. A new Low temperature plasma integration technology was developed by Zhongke Jingjing Environmental Technology Jiangsu Co., Ltd. in China and its dioxin emission reduction efficiencies were analyzed while equipped in medical waste incinerations. It was found that over 83% of toxic equivalent quantity dioxins could be removed with this technology. Dioxin emissions reduction characteristics of low temperature plasma integration technology were compared with other dioxin reduction technologies, which showed that it was highly conducive in dioxin control.

9CO.1**Mode Specified Semi-volatile Chemical Composition in PM Emissions from a Commercial Gas Turbine Aircraft Engine.**

ZHENHONG YU, Michael Timko, Andreas Beyersdorf, Luke Ziemba, Edward Winstead, Bruce Anderson, Scott Herndon, Richard Miake-Lye, *Aerodyne Research, Inc.*

It has been known that non-volatile particulate matter (PM) emissions from commercial aircraft engines can have significant impacts on local air quality and human health. NASA's Alternative Aviation Fuel EXperiment 1 (AAFEX 1) field measurement campaign was performed to characterize and quantify both volatile and non-volatile PM emissions from commercial gas turbine aircraft engines, with participants from eleven governmental agencies, universities, and companies.

In this study, we determined semi-volatile chemical compositions of nucleation/growth mode and soot mode particles in the engine exhausts at a variety of engine powers (4-100% thrust) with a compact time-of-flight aerosol mass spectrometer (C-ToF-AMS). Organic and sulfate components of both nucleation/growth and soot mode particles, were observed, while burning the conventional Jet-A fuel. Nitrate components in both the nucleation/growth and soot modes were negligible from the measurements.

Organic species were dominant at idle, but the sulfate content became important with increasing engine power. The organic composition of the nucleation/growth mode particles decreases with increasing engine power, and that of the soot mode initially decreases with increasing engine power, but then slightly increases again above 45% engine thrust, probably due to the increasing contribution from lubrication oil emissions. Our results demonstrate that the organic PM at idle is mainly aromatic species; while at 85% thrust, lubrication oil dominates.

This study implies that organic emission indices (EIs) from the nucleation mode particles decrease with increasing engine power, similar to the emissions of gaseous UHCs; and sulfate EIs from the soot mode particles strongly correlate with the black carbon soot emissions. These results show that an appreciable amount of semi-volatile PM can be generated in the exhaust plumes from a commercial aircraft engine. Thus, volatile PM must be studied as carefully as non-volatile soot emissions to fully address local air quality and human health impacts of aviation.

9CO.2**Predicting the Fuel Consumption and Tailpipe Emissions from Light-Duty Passenger Vehicles using Artificial Neural Networks.**

Shiva Tarun, Asher Zachary, Johnston Brian, Bradley Thomas, SHANTANU JATHAR, *Colorado State University*

There is growing evidence that on-road emissions from mobile sources exceed emissions determined during chassis dynamometer tests. In this work, we used a portable emissions monitoring system and artificial neural networks (ANNs) to measure and model on-road fuel consumption and tailpipe emissions from a Tier-2 light-duty gasoline and diesel vehicle. Tests were performed on at least five separate days for each vehicle and each test included a cold start and operation over a hot phase. Fuel consumption and emissions rates were calculated at 1 Hz using information gathered from the vehicle using the onboard diagnostics port and the PEMS measurements. We trained ANN models on part of the data to predict fuel consumption and tailpipe emissions at 1 Hz for both vehicles and evaluated these models against the rest of the data. The ANN models performed best when the training iterations were set to larger than 25 and the number of neurons in the hidden layer was between 7 and 9, although we did not see any specific advantage in increasing the number of hidden layers beyond 1. The trained ANN models predicted the fuel consumption over test routes within 10% and 3% of the measured values for the gasoline and diesel vehicle respectively. The ANN performance varied significantly with pollutant type and we were able to develop satisfactory models only for the diesel vehicle. The ANN models for NO_x were able to predict total emissions within 10% of the measured values. The ANN models performed better than multivariable regression models such as those used in mobile source emissions models (e.g., EMFAC). To highlight the value for real world driving, we evaluated the vehicle-specific ANN models to pick routes for lower fuel consumption or tailpipe emissions.

9CO.3

Secondary Organic Aerosol (SOA) Formation from a Light-Duty Gasoline Direct Injection (GDI) Vehicle at Different Drive Conditions. WEIHAN PENG, Niina Kuittinen, Cavan McCaffery, Stephen Zimmerman, Patrick Roth, Roya Bahreini, David R. Cocker III, Georgios Karavalakis, *University of California, Riverside*

Aerosol particle emissions from vehicular-related activities is important to particulate matter emission budget in urban areas. As emission control technologies for primary aerosols (PA) advance, secondary organic aerosol (SOA) becomes increasingly important. Unlike primary aerosol directly emitted to atmosphere, SOA forms from gas-particle partitioning of reactions products from VOCs, NO_x, and other species in atmosphere. Studies have shown SOA formation potential from GDI vehicles for select drive cycles (e.g. LA92, FTP). However, no comprehensive studies have characterized SOA formation at different drive conditions: aggressive and mild, hot- and cold- start. This work investigates the primary and secondary aerosol composition from a GDI vehicle when operated over 7 different drive cycles, including FTP, NEDC, LA92, US06, HWFET and two high-speed drive cycles developed by California Department of Transportation (Caltrans).

Emission samples were collected from a GDI light-duty vehicle operating California E10 fuel and atmosphere aging products were studied at the Mobile Atmospheric Chamber (MACH) at UC, Riverside/CECER. The particle size distribution, density, volatility and aerosol bulk chemical composition were analyzed. Both primary and secondary pollutants from this vehicle were compared between more and less aggressive cycles, hot- and cold- start cycles, to investigate the effects from cycle starting conditions and speed on SOA formation. Black carbon and ammonium nitrate account for the major fraction of tailpipe emission and chamber aging aerosol products respectively, when operated over all drive cycles in this study.

9CO.4

Aircraft Exhaust Nanoparticles: Great Contribution of Jet Engine Lubrication Oil. AKIHIRO FUSHIMI, Katsumi Saitoh, Yuji Fujitani, Nobuyuki Takegawa, *National Institute for Environmental Studies*

The global use of jet engine aircraft has been rapidly increasing. Effects of aircraft emissions on atmospheric compositions, including those of particulate matter (PM), are ubiquitously found from the ground level to the upper troposphere. A new PM emission standard for jet engines will come into effect in 2020. However, the chemical characteristics of aircraft exhaust particles, especially for size-resolved chemical compositions of nanoparticles, are poorly understood.

In this study, we show for the first time that organic compounds originating from jet engine lubrication oil is a major constituent of nanoparticles (diameter <30 nm) emitted from aircraft. Using a highly sensitive analytical method, including thermal-desorption gas chromatography/mass spectrometry (TD-GC/MS), we identified unburned, nearly intact forms of lubrication oil as a major component of nanoparticles emitted from in-use commercial aircraft under real-world conditions.

Our findings have an important implication for emission control strategies and health risk assessments. While lubrication oil is necessary for jet engines, the contribution of lubrication oil to aircraft exhaust nanoparticles has not been evaluated quantitatively. The development of superior control technologies for oil emissions may greatly reduce aircraft exhaust nanoparticles. Reducing oil contributions is beneficial in mitigating the health risks of aircraft exhaust nanoparticles, as jet lubrication oils contain some toxic materials. Our findings also have an implication for climate issues. Detailed knowledge of aircraft emissions is important for improving our understanding of the origin and fate of ambient particles in the upper troposphere, which can potentially affect the radiative balance of the atmosphere.

Related publication:

Fushimi A., Saitoh K., Fujitani Y., Takegawa N. (2019) Identification of Jet Lubrication Oil as Major Component of Aircraft Exhaust Nanoparticles, *Atmos. Chem. Phys. Discuss.*, <https://doi.org/10.5194/acp-2018-1351>.

9CO.5**Diesel Exhaust Particle Number Measurement and Measurement Variability Using Off-Highway Test Cycles.**

KIRBY J BAUMGARD, Nicholas J Barsic, *John Deere Power Systems*

Tailpipe particle number (PN) emission limits for European heavy-duty diesel engines have been introduced as part of the off-highway Stage V regulations. The regulations state that PN must be measured from either an approved partial flow dilution system or a full flow dilution system [EU 2016/1628]. This paper investigates: 1) ideal particle sampling probe location for the Sierra BG3 partial flow dilution system, 2) compares steady-state PN measurements for both CVS and BG3 systems, and 3) compares NRTC, non-road transient test cycle, and RMC, ramped modal cycle, data between CVS and BG3 systems.

The initial sample probe location was immediately downstream of the BG3 mini-dilution tunnel. PN results suggested that particles were not fully mixed at that location so the probe was moved downstream after the cyclonic separator. PN diluted by the BG3 and measured after the cyclonic separator resulted in good agreement with PN measured in the exhaust pipe with a second APC.

To compare the particle number emissions from the BG3 system to the CVS system, an exhaust sample was diluted with the BG3, passed through the cyclonic separator and then sampled with APC #1. Simultaneously, a second APC sampled from the CVS dilution system. A total of 133 data points were measured with and without a DPF and therefore, the PN concentration range varied from 1×10^{10} to 1×10^{14} #/cm³. Using a Pierson's correlation analysis, the BG3 PN values were typically within 2% of the CVS values.

Repeated NRTC and RMC tests indicated that CVS and BG3 system %COVs were less than 1.5% and 7.5%, respectively. PN Comparisons between the CVS and BG3 for the NRTC and RMC cycles were typically within 10%. These values were measured without exhaust aftertreatment.

9CO.6**Characterization of Smoke for Spacecraft Fire Safety.**

XIAOLIANG WANG, Hao Zhou, W. Patrick Arnott, Marit Meyer, Samuel Taylor, Hatef Firouzkouhi, Hans Moosmuller, Judith Chow, John Watson, *Desert Research Institute*

Fire is among the most catastrophic threats to space activities. Conventional spacecraft smoke detectors are not optimized for detecting space smoke, which differs from that on Earth due to differences in fuel materials, burning conditions, and particle formation/transformation processes as well as lack of gravity. This study characterizes smoke from combustion of spacecraft-relevant materials with an aim to improve space fire detection. Three spacecraft-relevant materials, cotton lamp wick, Poly(methyl methacrylate) (PMMA), and Nomex[®] fabric were burned in smoldering and flaming conditions. A suite of instruments was used to characterize gas and particle emissions, including carbon monoxide, carbon dioxide, volatile organic compounds, particulate matter mass, particle size distribution, light scattering and absorption, and particle chemical composition. Particles emitted from flaming PMMA were fractal-like soot agglomerates, different from the near spherical particles found for other fuels and burning conditions. Particles from smoldering cotton combustion had a bimodal number size distribution, while those from other fuels and test conditions exhibited mono-modal lognormal number size distributions. Smoke particles from flaming PMMA combustion were black with single scattering albedos < 0.3 , while particles from other burned materials demonstrated low light absorption, with single scattering albedos > 0.9 at 405-781 nm. Mass extinction coefficients were $6.4 \text{ m}^2/\text{g}$ for flaming PMMA and $2.2\text{-}3.5 \text{ m}^2/\text{g}$ for smoldering combustions at 632.8 nm. Carbon monoxide and particulate matter mass emission factors were higher for smoldering than for flaming combustions, while carbon dioxide emission factors were higher for flaming combustions. These data are of essence for optimizing spacecraft smoke detector designs. They are also useful for numerical modeling of smoke emission and transport.

9CO.7

Black Carbon and Particle Size Distributions Emitted from a Modern Aircraft Turbofan Engine Operated on Sustainable Alternative Jet Fuels. JOEL CORBIN, Prem Lobo, Gregory Smallwood, Tobias Schripp, Ewan Crosbie, Michael Shook, Claire Robinson, Edward Winstead, Bruce Anderson, Richard Miake-Lye, Zhenhong Yu, Andrew Freedman, Philip Whitefield, *National Research Council Canada*

Emissions from aviation related activities are a unique source of pollution in the urban environment and at cruise altitudes. Efforts are underway worldwide to reduce the environmental impacts of aviation through the use of sustainable alternative jet fuels (SAJFs). To date, alternative fuels blended with conventional Jet A/Jet A-1 (up to 50%) have been approved for use in the commercial aviation sector and have been shown to dramatically reduce black carbon (BC, or non-volatile particulate matter, nvPM) emissions. However, limited information is available on the physical, chemical, and optical properties of BC from modern turbofan engines burning SAJFs. If these properties vary, then the response of different instruments, which measure PM based on different properties and physical principles, may vary.

In this study, we measured the ground-level emissions of a V2527 engine, mounted on the DLR A320 ATRA research aircraft burning two conventional jet fuels and three blends of conventional jet fuel and SAJFs. The emissions were then distributed via a sampling manifold to a suite of instruments measuring black carbon (BC), particle size distributions (PSDs), and particle optical properties. BC was measured as refractory BC (rBC) by three pulsed laser-induced incandescence instruments (LII300); as equivalent BC (eBC) by two instruments using the extinction-minus-scattering principle (CAPS PMssa), two using the photoacoustic principle (PAX and MSS), and two using the filter-based attenuation principle (PSAP and TAP). PSDs were measured by three scanning mobility particle sizers (SMPS) and two electrometer-based particle sizers (EEPS and DMS500) as either total or non-volatile size distributions. We discuss the consistency between this comprehensive suite of measurements. The mass concentrations derived from the BC instruments were generally close to the median measurement, with the exception of the PSAP and TAP. Quantitative comparisons will be discussed between these instruments and the measured PSDs.

9CO.8

Soot Formation Models for Non-Premixed Flames with Variable Stoichiometric Mixture Fraction and Strain. PHILLIP JOHNSON, Rajan K. Chakrabarty, Benjamin M. Kumfer, *Washington University in St. Louis*

Many soot formation models were developed for a particular application with unique characteristic mixing times and/or validated under fuel-air combustion conditions only. Therefore, their use in different contexts, such as oxy-combustion, can lead to inaccurate predictions. A soot-producing flame can become non-sooting (blue) with an increase in Z_{st} , even while maintaining constant flame temperature, or through increasing strain rate. In this study, twelve semi-empirical soot models were evaluated on their ability to respond to changes in Z_{st} and strain in a series of counterflow flames which span the experimental sooting-to-non-sooting transition.

All current semi-empirical models failed to predict a blue flame for increased Z_{st} . Two current semi-empirical models predicted a blue flame for increased strain. No existing model came within an order of magnitude of its predicted soot volume fraction target for both evaluations. A new semi-empirical model that is currently in development was also evaluated which uses only one equation and does not require complex gas chemistry. Despite its simplicity, preliminary results show that this model was able to predict a blue flame for both evaluations.

9CO.9

Influence of Temperature and Dilution on Final Soot Nanostructure. JUSTIN DAVIS, Igor Novosselov, *University of Washington*

Morphological evolution of nascent to mature combustion-generated particles is of interest due to changes in particle optical properties, density, chemical composition, and their effect on human health. In this work, the nanostructure of primary soot particles is investigated using argon dilution in laminar ethylene, ethane, and methane flames. A co-flow reactor oriented downwards allows for precise control on combustion conditions due to increased flame stability brought on by competing buoyant and convective forces. The dilution is varied from 0% to 90% by volume to investigate particle formation in temperature ranges from 1650 to 1950 K. High-resolution transmission electron microscopy displays different levels of particle maturity, from young soot with minimal order to mature particles with a core-shell nanostructure. A novel image processing algorithm helps to quantify differences in soot nanostructure. Graphene-like flakes that comprise young and mature soot particles are around the same size, indicating the molecular weight of PAHs is similar for young and mature soot. However, the graphene-like flake curvature decreases and the percentage of stacked fringes increases significantly for high temperature (low dilution) flames. The reduction in curvature suggests the more planar PAHs have greater C/H ratios, independently verified by total organic carbon analysis. Overall, this study suggests the driving factor of soot maturity is a reduction in steric hindrance due to carbonization kinetics at high flame temperatures. These results can be used for validation of soot modeling approaches and to improve the understanding of structural changes as soot particles traverse the flame front.

9CO.10

A Multiscale Study of Soot Morphology and Evolution in Combustion Devices. KHALED MOSHARRAF MUKUT, Eirini Goudeli, Somesh Roy, *Marquette University*

Soot morphology is an important factor which affects the aging of soot particles in and outside of a combustion device. The current study investigates potential effects of different factors such as temperature, pressure, exhaust gas recirculation (EGR), etc. on soot morphology in a high-pressure spray combustion configuration. A stochastic soot model is used to model the soot formation in engine combustion network's (ECN) constant volume combustion chamber with n-dodecane fuel. The soot aggregates are quantified by different parameters such as surface area, volume, fractal dimension, collision diameter, C/H ratio, etc. at different locations during different stages of combustion to investigate the morphological evolution of soot particles. Different stages of soot formation will also be investigated from a first-principal point of view using reactive molecular dynamics simulations. The results from combustion CFD at the device scale and molecular dynamics at microscale will be carefully analyzed and compared to gain a better understanding of the process of soot evolution in combustion devices.

9CO.11**Ash Formation in High Pressure Oxy-Combustion Systems.**

DISHANT KHATRI, Zhiwei Yang, Richard Axelbaum, *Washington University in St. Louis*

The Pressurized Oxy-Combustion (POC) process is receiving tremendous amount of attention as it is regarded as the technology for reducing CO₂ emissions with possibly increase in the total efficiency over atmospheric oxy-combustion. Although a promising technology for power generation, the impact on pollutants, such as the particulate matter (ash) has not yet been established at higher pressures. Therefore, in this work, the formation and evolution of fine ash particles will be evaluated in a pressurized oxy-combustor designed for a new POC technology staged pressurized oxy combustion (SPOC). The coal is fed dry using a screw feeder. A three stage high pressure sampling dilution system is designed to take the ash sample at the bottom of the pressurized combustor. The effect of pressure on ash formation is understood by varying the pressure of the system from 1 to 15 Bar. The effect of firing rate is understood by keeping pressure constant but changing the thermal input from 50 KW to 100 KW. The particle size distributions were measured using a Scanning Mobility Particle Sizer and an Electrical Low Pressure Impactor. The impactor also collected ash samples for the Scanning Electron Microscope and Energy-dispersive X-ray Spectroscopy to analyze size-segregated compositions. The experimental data, along with analytical models will help to understand the observed trends during these studies.

9CO.12**Emission Factors and Physicochemical Properties of Soot**

Produced in Low-Temperature Combustion. OMAR EL HAJJ, Khairallah Atwi, Zezhen Cheng, Alanna L. Koritzke, Matthew G. Christianson, Brandon Rotavera, Rawad Saleh, *University of Georgia*

Low-temperature combustion has emerged as a promising strategy for reducing pollutant formation in vehicle emissions. While unveiling the differences in ignition chemistry between low-temperature and conventional high-temperature combustion is an active area of research, there is limited understanding of how these differences affect soot formation and its physicochemical properties. Here, we conducted combustion experiments controlled at a constant equivalence ratio and at temperatures varied in a stepwise fashion between 500 K and 1200 K. We performed real-time measurements of soot emission factors using a scanning mobility particle sizer, light-absorption properties using a photoacoustic instrument, and volatility using a thermodenuder. We also collected samples for offline chemical analysis. To illustrate the importance of the fuel chemical structure in dictating soot formation in low-temperature combustion, we used two structurally different model fuels, iso-octane and cyclohexane. Soot emission factors in iso-octane combustion dropped rapidly with decreasing temperature, completely disappearing at temperatures lower than 1000 K. On the other hand, while cyclohexane combustion exhibited a soot formation behavior at high temperatures that was similar to iso-octane, it featured a resurgence in the low-temperature regime (~600 K), with emission factors of the same magnitude as at 1200 K. These findings are consistent with ignition-time simulations, which show a steady decrease in iso-octane reactivity with decreasing temperature, while the decrease in cyclohexane reactivity with decreasing temperature is interrupted by a sharp increase at 600 K. Notably, we observed stark differences in physicochemical properties between high-temperature soot (HTS) and low-temperature soot (LTS) in cyclohexane combustion: 1) the molecular sizes of LTS (< 200 Da) were smaller than HTS (300-3000 Da), 2) LTS was an order of magnitude less absorptive than HTS in the visible spectrum, and 3) LTS was more volatile than HTS.

9IA.1

Fungal Communities in Puerto Rican Homes after Hurricane Maria. JUAN PEDRO MAESTRE, Filipa Godoy Vitorino, Benjamin Bolaños-Rosero, Felix Rivera-Mariani, Humberto Cavallin, Kerry Kinney, *University of Texas at Austin*

The slow rebuilding and recovery efforts in the aftermath of Hurricane Maria in Puerto Rico may have led to fungal proliferation in many homes with minimal abatement. The respiratory health impact of these conditions is of great concern, particularly with respect to chronic inflammatory respiratory conditions such as asthma. In this study, the microbial communities of 50 homes located San Juan, are under scrutiny over a 2-year period, 25 homes affected by hurricane-associated flooding and 25 homes not affected. Airborne dust samples were collected using settled dust collectors indoors and outdoors, vacuuming floors, and swabbing door trims (indoor and outdoor). DNA from dust samples was extracted with PowerSoil kit, analyzed via high-throughput sequencing targeting the ITS rRNA gene. The pro-inflammatory potential (PIP) of indoor air samples collected is also being evaluated through quantitative assessment of induced pro-inflammatory cytokines in peripheral human blood.

Results collected to date indicate that home environment factors such as pet ownership, and smoking are not associated with higher house dust PIP. However, homes whose interiors were flooded during the hurricane, damage to the kitchen area and poor ventilation are associated with a 1.2 ($p = 0.009$) and 2.35-fold ($p = 0.03$) increase in the dust PIP. Similarly, flooding damage that required removal of floors, roof, or wood is associated with an increase in the dust PIP ($p = 0.02$ to 0.004). Higher relative abundances of moisture-associated fungi were found indoors compared to outdoors, with relative abundances up to 50%. The moisture-associated genera *Trichoderma*, *Aspergillus*, *Fusarium* and *Wallemia* were found frequently indoors. These results suggest that indoor conditions that result from long-term, unrepaired flood damage, may promote moisture-associated fungal taxa and increase the risk of occupant exposure to particulate matter with higher pro-inflammatory potential.

9IA.2

Aerosol Movement and Deposition into Hidden Interior Spaces Within a Full-Scale Test House. MENGJIA TANG, Ningling Zhu, Kerry Kinney, Atila Novoselac, *University of Texas at Austin*

Hidden, unmaintained spaces within buildings serve as reservoirs for particulate matter that may become resuspended during occupancy. While previous research has examined how particles from hidden areas such as wall cavities and crawl spaces can move into a building, much less is known about aerosol transport to hidden interior spaces. The objective of the current study was to measure the transport of indoor aerosols generated in one room to a variety of hidden interior spaces including closets, cabinets and drawers. To this end, a series of seven aerosol ($3.2 \mu\text{m}$ fluorescent particles) and tracer gas injection experiments were completed in a 120 m^2 full-scale test house. The movement and deposition of the traceable particles in the open visible spaces as well as the hidden interior spaces were determined using a fluorescent stereoscope to quantify the concentration of particles collected on glass slides placed throughout the house. An additional six tracer gas experiments were also completed to measure the circulation between selected indoor hidden spaces and the surrounding rooms. The results of the study indicate that the injected particles were deposited on horizontal surfaces throughout the house in both the open and hidden spaces. While the particles readily penetrated into closets with closed doors, at least one percent of the injected aerosol penetrated into more sealed spaces such as closed drawers within closed cabinets. Interestingly, air and particle movement between the hidden spaces and adjacent rooms were unaffected by mechanical ventilation. Temperature differences (e.g., buoyancy forces) may be an important contributor to the movement of air and particles into and out of hidden spaces but additional studies will be required to elucidate these factors further.

9IA.3

The Impact of Cooking Pan Material on Ultrafine Particle Emission Rates. MEHDI AMOUEI TORKMAHALLEH, Hamed Sharifi, Maryam Dareini, Giorgio Buonanno, *Chemical and Aerosol Research Team, Nazarbayev University*

Previous studies demonstrated that cooking is one of the major sources of indoor UFPs. It is important to focus on different cooking components to identify the most influential source which controls the overall cooking UFP emissions. This identification may then create opportunities to reduce cooking emission. Oil, meat, stove and pan are among the key sources contributing to cooking PM. It was found in the literature that desorption of semivolatile organic compounds (SVOCs) from the heated metal surfaces including pans and burners contributes to UFP emissions. Thus, the material coated on the surface of the pans may impact the amount of surface deposited SVOCs, and therefore the UFP emission rate. Among different cooking components, the emission rate of UFP generated from a heated cooking pan itself has not been yet investigated. The aim of this study is to examine the impact of type of cooking pans including Teflon, aluminum, ceramic and granitium pans on UFP emission rates under controlled experimental conditions. The four pans were exposed to indoor air under the same conditions for 24, 48, 96 and 144 hours and then were heated for 10 minutes while the temperature of the pan was recorded. After the 10 minutes heating, the pan was removed from the experimental chamber to start the particle decay period. Furthermore, this study investigates the relationship between the pan exposure time to indoor air prior to heating and the UFP emission rates during the heating. Total particle number emission rates from heated pans are estimated using an Aerasense (Netherlands) NanoTracer capable of quantifying particle number concentration up to 10^6 particles/cm³ for UFPs down to 10 nm. While the experiments are being conducted, the primary results showed that after 24 hour exposure to indoor air of a kitchen, Ceramic and Teflon pans produced 3.6×10^{13} and 1.29×10^{12} particles/h, respectively. When Ceramic pan was exposure to indoor air for 96 hours no significant changed was observe in UFP emissions rate (2.65×10^{13} particles/h) while it increased to 1.4×10^{14} particles/h for 144 hour exposure time. More results will be presented during the AAAR 37th annual conference.

9IA.4

Occupancy Sensing with Chair-Embedded Thermocouples: Applications for Evaluating Human-Associated Bioaerosol and VOC Emission Factors. DANIELLE WAGNER, Aayush Mathur, Brandon E. Boor, *Purdue University*

Human occupants in office environments are an important indoor source of bioaerosols and volatile organic compounds (VOCs). Concentrations of human-associated bioaerosols and VOCs are strongly linked to occupancy patterns. Reliable methods for counting occupants in an indoor space must be implemented in order to determine per-person bioaerosol and VOC emission factors (no. or $\mu\text{g h}^{-1}$ person⁻¹), thereby improving our understanding of how occupants shape the composition of indoor air. Occupancy sensing inferred from carbon dioxide measurement or bi-directional door sensors are subject to uncertainties. The objective of this study is to evaluate a new sensing technique to precisely determine spatiotemporal occupancy patterns in an office through use of chair-embedded thermocouples.

Occupancy was tracked for six months in the Herrick Living Laboratories at Purdue University, which are four modern open-plan offices with precisely controlled HVAC systems. One office with a twenty desk capacity was evaluated. A K-type thermocouple was securely mounted to each chair cushion surface and connected to a portable USB data logger. The seat temperature was detected every 15 seconds. An algorithm was developed to identify rapid surface temperature shifts corresponding to changes in chair occupancy. A seated individual counts toward occupancy, whereas an empty seat counts as zero; thus an error is introduced for those standing in the room for short periods. The count was summed for all twenty chairs to calculate the number of people in the room with 15-second time-resolution.

The chair-embedded thermocouples were integrated with real-time measurements of bioaerosol and VOC concentrations to estimate per-person emission factors over time. Daily and weekly trends in occupancy were determined for the office. Spatial occupancy maps were created to visualize the location of emission sources. The mapping allows for insight into whether pollutant origins are from multiple additive or single human sources. This method of occupancy detection is most effective in spaces where people are usually seated, such as offices and classrooms. Being able to more accurately denote the relationships between occupants and resulting concentrations of bioeffluents can inform exposure studies and ventilation control strategies.

9IA.5

Insights on Particulate Matter Formation and Evolution during a 3D Printer Operation. SAMEER PATEL, Sumit Sankhyan, Marina Vance, *University of Colorado Boulder*

Owing to a range of factors such as advancement in technology and increased affordability, three dimensional (3D) printers are gaining attention as a consumer product. Depending on the model and operating conditions, these 3D printers can lead to high exposure levels of ultrafine particles (UFPs) and volatile organic compounds (VOCs). Research efforts have been gaining impetus to add to our nascent and, therefore, limited understanding of the characteristics, interaction with surroundings, and health effects of 3D printer emissions. Another sparsely explored topic is the fundamental aerosol dynamics underlying particulate matter formation and growth during 3D printer operation which is limited by instrumentation capability to measure the lower end of the particle size distribution.

We characterized particle size distributions, optically absorbing particulate matter (PM), and total non-methane hydrocarbon emissions from a 3D printer in a chamber using a 1-nm SMPS, five wavelength aethalometer, and a flame-ionization detector, respectively. Effects of filament type on PM characteristics, emission rates, and emission factors were established. A numerical model for particle formation (via nucleation) and growth was applied to the experimental data for the estimation of the physical parameters of the semi-volatile emissions from different types of filaments. Numerical analyses to investigate links between the measured total hydrocarbons and PM was also conducted. Lastly, model results were used to estimate PM levels and resultant exposure when the same 3D printer is used in built environments with varying physical and ventilation characteristics.

9IA.6

Exposure to Endotoxin in a Cohort of Pregnant Women and Their Children. Javier Ustariz, HECTOR JORQUERA, Arturo Borzutzky, *Pontificia Universidad Catolica de Chile*

Endotoxin is a lipopolysaccharide component of the outer membrane of gram-negative bacteria, associated with pro-inflammatory responses in the respiratory system. Endotoxin has been linked to allergies and asthma both in children and adults. In urban environments, indoor concentrations of endotoxins tend to be higher than outdoor ones, owing to inefficient ventilation and presence of indoor sources.

Endotoxin in house dust is a good indicator of long-term indoor exposure. This cohort study aims to determine prenatal and perinatal conditions, as well as other biological and environmental factors that may contribute to the risk of developing allergic diseases and/or asthma in the offspring, and might provide enough information on the subjects to prevent it or treat it in the future.

We have started to recruit a cohort of 250 pregnant women in Santiago, Chile. Two periods for household sampling have been set, between weeks 24-30 of the pregnancy and between weeks 14-20 after childbirth. Indoor dust has been sampled using an Indoor-Biotechnologies Dustream™ Collector. Endotoxin has been quantified by using the Limulus Amebocyte Lysate Kinetic-QCL test kit (LAL Kinetic-QCL). Other indoor parameters monitored are humidity, CO₂, CO, NO₂ and O₃ for 5-8 days within the aforementioned periods. To assess perinatal outdoor exposure to ambient air pollution, we will collect data from the monitoring station closest to the family's home for the whole study period.

House dust collection and indoor air quality monitoring began in January 2019. The first baby of the cohort was born in February 2019. Preliminary results of this cohort study will be presented for endotoxin and indoor pollutants; for the latter, comparison with ambient air quality monitoring will also be discussed.

9IA.7

Computational Fluid Dynamics Modeling of Particles on the International Space Station. KAITLYN KOEHLER, Andrea Ferro, Goodarz Ahmadi, *Clarkson University*

Particles behave differently on the International Space Station (ISS) than they do on Earth. On Earth, particles deposit due to gravitational settling, but this is not the case on the ISS due to the microgravity conditions. A computational fluid dynamics (CFD) model has been developed in ANSYS-Fluent to study the flow of particles in the US Laboratory of the ISS. This model can be applied to predict astronauts' exposure to particulate matter (PM). Sources of PM are modeled using data from the analysis of dust taken from the air filters on the ISS. The analysis of the dust was conducted at Clarkson University and other Universities participating in the Diverted Unwanted Space Trash (DUST) program. In addition to assessing exposure to particles, the CFD model of the US Laboratory is used to study smoke/pyrolysis particles dispersion in the presence of a heat source for application to fire detection on the ISS. The quick detection of fires on the ISS is critical to the safety of the station and its crew. The current fire detection system on the ISS was designed based on the knowledge of terrestrial fires. On Earth, smoke rises due to buoyancy forces, but this is not the case on the ISS due to the lack of gravity. Therefore, the dispersion of smoke particles on the ISS is controlled by other mechanisms such as turbulent diffusion and the airflow due to ventilation conditions. Using the CFD model as a source-to-receptor model for smoke/pyrolysis particles can provide information for the optimization of the fire detection system on the ISS.

9IA.8

Characterisation of SVOCs Derived from Indoor Cooking and Cleaning Activities. Elizabeth Lin, Marina Vance, Delphine K. Farmer, KRYSTAL GODRI POLLITT, *Yale University*

Pollutant emissions from cooking and cleaning activities as well as use of personal care products are major contributors to personal exposure in the indoor environment. The HOMEChem study (House Observations of Microbial and Environmental Chemistry) was conducted to better understand these indoor exposures. During June 2018, real-world cooking activities (stir fry) as well as cleaning activities with terpene- and chlorine-containing products were conducted in the University of Texas at Austin's test house. Each cooking and cleaning activity was sequentially repeated over different study days to facilitate comprehensive characterisation of individual activities. Layered experiments with multiple different cooking and cleaning activities over a study day were also performed to mimic real-world indoor behaviour patterns and exposure profiles. As part of the larger HOMEChem study, exposure levels to semi-volatile organic compounds (SVOCs) were measured using a low-cost air pollutant sampling device. This sampler was deployed in the kitchen of the test house for each of the sequential and layer experiments and passively absorbed SVOCs into a polydimethylsiloxane sorbent matrix. At the end of the study period, the polydimethylsiloxane samples were analysed off-line by thermal desorption high resolution gas chromatography time-of-flight mass spectrometry. Twenty-four-hour averaged concentrations of 36 SVOCs were quantified for each experiment day. Unique exposure profiles were identified for each cooking and cleaning activity. Correlations between SVOCs were evaluated using heat maps for layered activity experiments. The principal components derived from this correlation analysis will be presented.

9IA.9

Laboratory Determination of the Functional Range of Eight Low-Cost Particle Sensors and Consumer Device. YANGYANG ZOU, Matthew Young, Melissa Ryan, Andrew May, Jordan Clark, *The Ohio State University*

Low-cost particle sensors are rapidly gaining popularity for monitoring human exposure to particulate matter (PM). Manufacturers of these sensors typically provide either effective or maximum range of concentrations over which the sensors are accurate. Evidence suggests the sensors' performance over this range can vary, and clear definitions of functional range can help understand this variance. This is especially true for indoor environmental monitoring.

To this end, we sought to understand potential limitations of the sensors in terms of their functional range. We conducted laboratory experiments using PM sources including burning incense and toast, and atomization of ammonium sulfate. Particle mass concentrations in these experiments ranged from near zero to over 1000 $\mu\text{g}/\text{m}^3$. We conducted linear regression analysis between the sensors and co-located reference instruments. From this we suggest methods to define upper and lower bounds of functional range. We found that: 1) there exists a range of concentrations beyond which correlation of low-cost sensors to reference instruments drops considerably; 2) this range differs drastically for different sensors and different sources and can begin at concentrations above those of typical indoor environments; and 4) increasing the averaging time increased the R².

9IA.10

Use of Piezobalance to Determine Volatility of E-Cigarette Aerosol. LANCE WALLACE, Wayne Ott, Kai-Chung Cheng, Tongke Zhao, Lynn M. Hildemann, *US EPA (retired)*

Some aerosols, such as nitrates, are volatile, and can escape from filters while being collected for gravimetric analysis. Recently e-cigarette liquids containing glycerin have become popular and their aerosol emissions appear to be volatile in part. Therefore collection by filters for gravimetric analysis might not provide useful data on density or source strengths. The Piezobalance (piezoelectric microbalance) provides a real-time measure of mass accumulating on its crystal surface. It can also quantify the mass leaving the surface due to volatilization. We present a general method for determining the fraction of mass that is volatilized as a function of time. After a source containing volatile material is turned on, the Piezobalance frequency increases from a baseline to a peak value, and then decreases as the crystal loses mass. The amount of the decrease divided by the amount of the increase over a period of time is the fraction $F(t)$ of the aerosol that is lost during that time. If the decay is followed long enough for the frequency to achieve an asymptotic (steady-state) value, then this ratio is the total volatile fraction F_{inf} . If we have a series of measurements of the observed fraction $F(t)$ at different times t , then we can fit an asymptotic curve of the form

$$F(t) = F_{inf}(1 - \exp(-t/\tau))$$

to estimate the two unknown parameters F_{inf} and time constant τ (time from the beginning of the decay period to reach $1 - 1/e$ of the final concentration). From 88 experiments, we find that the fraction (F_{inf}) of e-cigarette aerosol containing glycerin = 88% (SE 11%). The time constant $\tau = 16$ (SE 4) minutes. The method is general and can apply to other aerosol mixtures. One of particular interest is aerosol from marijuana liquid.

9IA.11

Investigating Aerosol Emissions from Cooking Oils. SUMIT SANKHYAN, Sameer Patel, Marina Vance, *University of Colorado Boulder*

Cooking is one of the main contributors to aerosol emissions in home environments. Cooking fumes, especially those produced by heating oils at high temperature, contain ultrafine and optically absorbing carbonaceous aerosols. These emissions have been linked to various respiratory and cardiovascular ailments.

The objective of this study was to investigate the aerosol emission rates from a variety of commonly used cooking oils with a range of smoke points using an electric heat source at various temperatures (below and above the smoke point). Oils tested include avocado oil, peanut oil, soybean oil, olive oil, coconut oil, and lard, each with and without the addition of salt. Air pollutant emissions were characterized in terms of particle size and concentration, relative concentrations of black and brown carbon (BC and BrC), and total non-methane hydrocarbons (TNMH).

Aerosol size distributions were characterized using a Scanning Mobility Particle Sizer (TSI) and an Aerodynamic Particle Sizer (TSI). Black carbon and brown carbon concentrations were investigated using a 5-wavelength aethalometer (Aethlabs). TNMH were measured using a flame ionization detector (Baseline-MOCON). Source apportionment of BC and BrC for different types of oil emissions was done using power-law fitting approach for angstrom exponent (α). Comparative analysis of oils in terms of PM, TNMH, BC and BrC content was done to put forward recommendations for oil usage based on cooking temperatures. This study will aid in bringing indoor air quality field measurements into perspective by isolating cooking emissions from other potential indoor sources.

9IA.12

Developing an Air Quality Index for Space Vehicles and Habitats. MEYTAR SOREK-HAMER, Marit Meyer, *NASA Ames Research Center, Moffett Field, CA, USA / USRA*

The development of an adequate tool to help the layperson understand pollution levels in their environment is of high importance. This tool must be able to inform about the levels of pollution in a simple and understandable way but also can be used for decision-making and mitigation activities to protect the health of the exposed population. One of the most useful and up-to-date approaches for characterizing air pollution is the Air Quality Index (AQI). It is an easily-calculated, powerful, data-driven tool that summarizes a complex phenomenon, such as air pollution, in straightforward indicators. The AQI system has been developed in different countries around the world, mainly for outdoor environments, based on the results of risk assessments, epidemiological studies, and current local air pollution regulations and standards. There is a need for such a system in low gravity indoor environments where air quality is of fundamental importance to astronaut health, with concerns encompassing both gaseous contaminants and particulate matter. Earth-based AQIs cannot be extrapolated to microgravity indoor environments due to different aerosol transport characteristics and altered lung deposition in low and partial gravity. The objectives of this work are to explore what areas of expertise, types of research, and data will be required to formulate a spacecraft-specific AQI. An initial dataset is available for this effort, combined from two aerosol sampling experiments, which have characterized airborne particulate matter on the International Space Station (ISS). We outline future research needs for formulating a narrowly focused version of a widely-used metric, namely, an indoor AQI for future space missions.

9IA.13**Indoor Environmental Quality and Association with Human Perception at Schools and Homes of Urban and Rural Areas.**HYEON-JU OH, Jong-Ryeul Sohn, *Korea University*

Poor indoor environmental quality (IEQ) poses a threat to respiratory health and interests in IEQ became increasing. Here, we investigated the indoor environmental quality at schools and homes of urban and rural areas and the survey on the human perception of IEQ was conducted. For the IEQ, the temperature, relative humidity, CO₂, bioaerosols, PM₁₀, PM_{2.5} levels and the variations of IEQ depend on the indoor potential sources (cooking and cleaning) were investigated, and their survey was conducted as the human perception, health performances and thermal comfort. There was no difference in PM₁₀ concentrations between urban and rural areas. However, PM_{2.5} showed significant differences between indoor and outdoor at urban areas. Higher correlation of PM levels between indoor and outdoor showed at the rural areas. There was no significant difference in the concentration of airborne bacteria and fungi between urban and rural areas. The CO₂ concentrations in schools were correlated with the corresponding the number of students (R² of 0.71- 0.85 in summer and 0.14 - 0.86 in winter). For the airborne bacteria and fungi, there was no significant difference in the concentrations of bacteria and their species between sampling places. However, for the concentrations of fungi, there was the significant differences in samples collected from urban and rural groups. Significant associations were observed between the satisfactions (%) of outdoor air quality and both indoor PM concentrations and respiratory illness symptom. This study shows that people's perception of outdoor pollutant concentration affects the satisfaction of indoor air quality concentration and the respiratory diseases and many sources in indoors may combine to become more serious problem together than they are separately. Also, this study demonstrated that human perception of outdoor pollutant level affects the satisfaction of IEQ levels.

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9IA.14**Ozone Reactions with Squalene: Particle Seeding and Formation.**BREANN COFFARO, Clifford Weisel, *Rutgers, The State University of New Jersey*

Particulate matter (PM) has been reported to form from the reaction of ozone and squalene, a natural component of skin oil. These particles contain carbonyls and organic acids, which can be potential respiratory and ocular irritants, so indoor exposures are of concern. A controlled reaction chamber was used to investigate the conditions that lead to particulate formation from squalene-ozone (SqO) reactions arising through nucleation mechanisms. Particle counts were analyzed with a TSI Condensation Particle Counter. Initial experiments with filtered background ambient air containing PM levels of 1,000-4,000 particles (#/cc) often resulted in the formation of an additional 5,000-10,000 #/cc about 20-60 minutes after the introduction of ozone during the spring and summer. During the fall and winter, particle formation was less consistent suggesting that the composition of the background particles is important in serving as nucleation sites. Spring and summer particles typically have higher organic content. An immediate large spike in PM counts (20,000 #/cc) was observed if new squalene was placed in the reaction chamber after the PM returned to background levels during the spring/summer, suggesting the presence of some residual organic nucleation particles. To further evaluate the role of nucleation in SqO particle formation, two sources of particles often present indoors were examined: PM formed by a heated nichrome wire and secondary organic aerosols formed from limonene and ozone. The nichrome wire particles, which are predominantly inorganic, did not result in particles produced from the SqO reaction while particles from the limonene ozone reactions resulted in formation of approximately 55,000 #/cc almost immediately after the introduction of the squalene. These results suggest that organic nucleation particles are an important component for the formation of particles from the reaction of ozone with squalene which influences indoor air counts and PM composition.

9IA.15

Assessment and Mitigation of Exhaled Electronic Cigarette Aerosols in a Multi-zone Indoor Environment. Li Zhang, Yan Lin, YIFANG ZHU, *University of California Los Angeles*

Electronic cigarettes (E-cigs) are battery-operated devices gaining increasing popularity as an alternative to tobacco cigarettes. To better understand the transport of exhaled e-cig aerosols and to evaluate the efficiency of various mitigation strategies, experiments were conducted in two neighboring laboratory rooms (one as Vaping Room and the other as Non-Vaping Room) under various conditions, including door segregation, enhanced ventilation and air filtration. A recruited e-cig user vaped in Vaping Room and particle number concentration (PNC) and $PM_{2.5}$ mass concentrations were measured concurrently in both rooms before, during and after the vaping activity. Secondhand exposure to exhaled e-cig aerosols was observed in this study. Transport of particle number from exhaled e-cig aerosols was observed from Vaping Room to Non-Vaping Room whereas almost no transport of $PM_{2.5}$ was observed. The transport process could be effectively mitigated by controls, especially for door segregation, where particle levels were reduced from 48% to 6%. Other controls, including enhanced ventilation and air filtration, increased particle removal efficiency in the room. Particle decay due to room air exchange rate (AER) was the primary contributor compared with decay due to aerosol dynamics (including processes of particle evaporation, surface deposition and coagulation).

9IA.16

A Dynamic Method to Measure Partition Coefficient and Mass Accommodation Coefficient for Gas/Particle Interaction of Phthalates in Indoor Environments. Jianping Cao, CLARA EICHLER, Yaoxing Wu, John Little, *Virginia Tech*

The particle/gas partition coefficient K_p and the mass accommodation coefficient α are two parameters characterizing the gas/particle interaction of semi-volatile organic compounds (SVOCs). Most of the available methods for measuring K_p require equilibrium at the chamber outlet, implying substantial preliminary testing. The need to separate gas- and particle-phase SVOCs also reduces method accuracy. Few studies measuring α for indoor-related SVOCs are available, and they usually ignore the wall loss of SVOCs, resulting in reduced measurement accuracy. To overcome these deficiencies, we developed a dynamic method coupling a laminar flow tube chamber and an SVOC mass transfer model. Using the interaction between gas-phase di-2-ethylhexyl phthalate (DEHP) and $(NH_4)_2SO_4$ particles (with diameters in the range of 10-600 nm) as an example, experiments were performed to evaluate the effectiveness and accuracy of the dynamic method. For the experimental conditions investigated (temperature = 25 °C and relative humidity < 10%), gas-particle interaction between DEHP and $(NH_4)_2SO_4$ particles is governed by surface adsorption because $(NH_4)_2SO_4$ particles are in solid state. In this case, gas-particle partitioning should be characterized by the surface-area-normalized partition coefficient (K_{pA}). K_{pA} and α were measured to be 260 ± 80 m and 0.20 ± 0.05 , respectively. Both are consistent with results reported in literature. The method applicability for other SVOC-particle combinations and the improvement of method accuracy require further study.

9IA.17

Particle Size: A Missing Factor in Risk Exposure to Toxic Metals in Indoor Aerosols of South-East Asia. HIMANSHI ROHRA, Ajay Taneja, *DR. B.R.A. University, Agra, India*

The work presents the investigation of indoor air pollution through analysis of metal bound size-resolved aerosols (2.5-10, 1.0-2.5, 0.5-1.0, 0.25-0.5, 0.25-0.1 μm) in residential homes at Agra, a city in South East Asia. A cascade impactor with PTFE filters collected metal bound PM in coarse, fine and ultrafine PM ranges. The concentration levels of measured metals ranged as 9- 20% with lowest in coarse and highest in PM fraction with aerodynamic diameter less than 2.5 μm . Also, the crustal elements dominated coarse fraction whereas the ultrafine range showed relatively higher proportion of toxic elements. Identifying the metal concentration, Ca, Fe, Al, Mg, K - Group I elements (major) and Zn, Co, Ba, Cd, Cu, Mn, Cr, Pb, Ni in Group II (minor) elements. Interestingly, the sum of total metal concentration was observed higher in summers than winters unlike PM concentration that recorded higher concentration in winters. 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 $\text{PM}_{0.5-0.25}$) elucidating increase in aerosol enrichment to finest particle. Results of this study aid in establishing relatively small international elemental modality dataset that could be incorporated in the exposure and risk assessment of indoor aerosols.

9IS.1

Dynamics of Volatile Organic Compounds in a Living Laboratory Office and HVAC System. TIANREN WU, Danielle Wagner, Jinglin Jiang, Philip Stevens, Heinz Huber, Antonios Tasoglou, Brandon E. Boor, *Purdue University*

Indoor emissions of volatile organic compounds (VOCs) and their subsequent transformations in HVAC systems can strongly influence the composition and chemistry of indoor air. Humans are an important indoor VOC source. Human-associated VOC emissions include exhaled breath, skin secretions, personal care products, ozone-skin oil reaction products, clothing, and microorganisms. Selected VOCs, such as monoterpenes, can be precursors for indoor secondary organic aerosol formation. The use of proton transfer reaction time-of-flight mass spectrometry (PTR-TOF-MS) enables for characterization of time-dependent VOC dynamics driven by transient occupancy and building system operation. The objective of this study is to understand how occupancy and ventilation mode influence spatiotemporal variations in the composition and concentrations of VOCs in an office and HVAC system.

A one-month measurement campaign was performed from February-March 2019 at the Herrick Living Laboratories at Purdue University, which are four modern open-plan offices with precisely controlled HVAC systems. Time-resolved concentrations of VOCs were measured via PTR-TOF-MS for one office housing twenty graduate students. An automated multi-point sampling system was built to sample VOCs at eight locations throughout the HVAC system: office return air (x2), supply air (x2), pre-/post-filter bank, common area return air, and outdoor air. Seven ventilation modes were implemented.

Preliminary results demonstrate that humans are a prominent source of VOCs in an occupied office and concentrations of human-associated VOCs exhibit diel variations driven by occupancy. VOCs related to metabolic activity reached peak concentrations in mid-afternoon (e.g. methanol: ~ 25 ppb; acetone: ~ 10 ppb), while those related to personal care products present daily maxima in the morning (e.g. decamethylcyclopentasiloxane (D_5): ~ 0.2 to 2 ppb) and then decay throughout the day. I/O ratios exhibited variations among the many VOCs detected, ranging from ~ 1 for benzene to > 10 for isoprene. Spatial variations in VOC concentrations throughout the HVAC system were observed for all VOCs. Concentrations of some VOCs were found to decrease by ~ 5 to 20% across the HVAC filter bank, suggesting VOC removal via partitioning to deposited particles. The primary loss mechanism for indoor VOCs is ventilation, and the rate increased with increasing outdoor air exchange rate. VOC emission factors ($\mu\text{g h}^{-1} \text{ person}^{-1}$) and deposition rates to indoor and ventilation duct surfaces will be reported, along with results from positive matrix factorization (PMF) analysis. To evaluate the impact of indoor VOC emissions on atmospheric chemistry, office- and building-normalized VOC emission factors to the urban atmosphere will be estimated.

9IS.2

Identification and Quantification of Personal Care Product Emissions Indoors during Exercise by GC-Vocus PTR-ToF.

Zachary Finewax, Megan Clafin, Demetrios Pagonis, Andrew Jensen, Olivia Jenks, Brian Lerner, Shelly Miller, Jose-Luis Jimenez, PAUL ZIEMANN, Joost de Gouw, *University of Colorado*

Humans spend approximately 90% of their time indoors. However, most air quality research has focused on the outdoor environment. Previous research has shown that the volatile organic compound (VOC) concentrations found in various indoor environments are comparable to polluted cities and megacities, and a significant fraction of these VOCs comes from application of personal care products. These products are known to be significant sources of monoterpenes, cyclic siloxanes and oxygenated VOCs that efficiently form secondary organic aerosol (SOA) through gas phase reactions with ozone and OH radicals. For various reasons, the speciation of monoterpenes and other oxygenates is not fully included in the chemical inventory, making it difficult to constrain SOA formation from personal care product emissions indoors and outdoors.

To address these and other issues, the ATHLETIC Indoor Campaign was conducted in the Dal Ward Athletic Center at the University of Colorado, Boulder from November 1 – 19 2018. A Vocus PTR-ToF was deployed to measure VOCs released from student athletes exercising in the weight room. The Vocus was either sampling the room continuously at 1 second time resolution or equipped with a GC to separate and identify product ion signals. The Vocus measurements alternated measuring the weight room and supply air on a 5-10 minute interval to determine the VOC enhancements within the room.

Monoterpenes, cyclic siloxanes, and oxygenated VOCs were identified and quantified. These emissions were determined to come from personal care products, as they displayed a different temporal profile than common VOCs from breath, such as acetone. Personal care product emission rates were highest during the morning workouts, consistent with patterns of showering or applying deodorant after waking. The speciation of monoterpenes to better constrain SOA formation indoors by reaction with ozone will be discussed.

9IS.3

Seasonal and Regional Variations of Indoor Organic Aerosol Water Content, Phase State, and Temperature-Based Partitioning.

BRYAN CUMMINGS, Manabu Shiraiwa, Peter DeCarlo, Michael Waring, *Drexel University*

Gradients in temperature and relative humidity (RH) arising from outdoor-to-indoor air transport impact organic aerosol (OA) water content, phase state, and gas-to-particle partitioning. We explored these parameter impacts using an indoor 2D-VBS aerosol chemistry model that predicts indoor OA concentration with contributions from outdoors, indoor emissions, and secondary OA formation. Inorganic aerosol is predicted from outdoor-to-indoor transport. Building parameters were set by distributions representing U.S. residences. A seasonal and regional dataset spanning 16 U.S. climate zones informed outdoor climatic (temperature, RH) and pollution parameters (organic and inorganic aerosol concentrations, composition). The 2D-VBS constrains OA O:C, informing OA hygroscopicity. Using organic and inorganic aerosol composition, aerosol liquid water (ALW) was predicted using κ -Kohler theory. Indoor RH drives ALW, and regional and seasonal conditions impacted indoor RH and thus ALW. Ratios of indoor ALW to dry particle mass reached ~ 0.4 in hot/humid climates during summer, while values largely remained < 0.1 year-round for arid climates and during winter in most regions. The ALW associated with OA was used to compute OA phase state (liquid, semisolid, amorphous solid). Residential OA most likely exists as a semisolid. However, certain hot/humid conditions yield liquid indoor OA, while indoor OA may be amorphous solid in cold or arid climates. These trends imply that partitioning of much indoor OA may have kinetic limitations inhibiting gas-to-particle equilibrium assumptions compared to residence timescales of indoor air, and that heterogeneous reactions may be slowed. However, using equilibrium partitioning assumptions, we predicted that ambient OA will generally condense as it goes indoors and encounters a greater absorbing mass of indoor-sourced OA. This effect will be exaggerated if indoor temperatures are colder than outside, but may be mitigated or reversed if the opposite is true.

9IS.4

Chemical Properties of Indoor Organic Aerosols. Hannah Przelomski, Erin Katz, Peter DeCarlo, RACHEL O'BRIEN, *College of William and Mary*

Indoor areas have larger surface area to volume ratios and slower air exchange rates compared to outdoors, thus increasing opportunity for aerosol particles to deposit onto indoor surfaces. The composition of this material can provide insights into transport and sources for indoor aerosol particles. The chemical composition and physical properties, including viscosity, may play an important role in the interactions between the indoor air and the lofted and deposited aerosol. Here, the chemical composition of the lower volatility fraction of aerosol particles collected in a kitchen is characterized using both ultra-high resolution mass spectrometry (UHR-MS) and offline-Aerosol Mass Spectrometry (AMS). The average molecular weight of these compounds is around 900 amu with an average carbon number of around 50. A comparison with online-AMS shows good overlap between the composition of surface film and aerosol particles generated by food cooking over the same time period. This organic mixture is also sensitive to aging processes including photolysis and ozonolysis. Here, a decrease in the average molecular weight is observed in both cases, consistent with fragmentation and volatilization of a fraction of the material. This work demonstrates the advantages of UHR-MS and offline AMS to characterize these particles. A better understanding of the composition and transformations of these films will provide insights into indoor chemical transport and exposure with impacts on human health in indoor spaces.

9IS.5

Phthalate Hydrolysis and Indoor Air Chemistry. DO YOUNG MAENG, V. Faye McNeill, *Columbia University*

Phthalic acid esters (phthalates) are abundant in indoor environments due to their widespread use in consumer products and building materials. Phthalates have been detected on indoor surfaces, in household dust, and in indoor air. Besides the adverse health effects of direct phthalate exposure, the degradation products of these species in the indoor environment pose additional health concerns. Phthalates are vulnerable to reaction with water molecules (hydrolysis) in the gas or aqueous phase, or on surfaces. The monoesters resulting from phthalate hydrolysis are often more potent endocrine disruptors than the parent molecule. Alcohols, the other main product of phthalate hydrolysis, may have an offensive odor and irritate eyes and respiratory system.

Our goal is to develop a numerical model of multiphase chemistry in the indoor environment that would enable us to quantify and predict the impacts of phthalates and phthalate hydrolysis on indoor air quality under different conditions. To this end, we are adapting the McNeill group model of aqueous atmospheric chemistry, GAMMA, to simulate multiphase processes on indoor surfaces. In order to more fully characterize the mechanisms and kinetics of phthalate hydrolysis under typical conditions, and to obtain required kinetic parameters for modeling, we have performed laboratory studies of phthalate hydrolysis in bulk aqueous solutions under a range of pH conditions. UPLC-QTOF MS/MS is used for detection of reactants and products. Experimental and preliminary modeling results will be presented.

9IS.6

Using Aerosol Principles to Advance Exposure Science: The Effect of Humidity on the Uptake of Water-Soluble Gases on Authentic Indoor Surfaces. MARC WEBB, Liyong Cui, Joanna Atkin, Glenn Morrison, Jason Surratt, Barbara Turpin, *UNC-Chapel Hill*

Surfaces play an important role in indoor chemistry, where surface area-to-volume ratios are greater than $3 \text{ m}^2/\text{m}^3$, orders of magnitude greater than typical of ambient aerosols. The surfaces of materials found in indoor environments are known to be soiled with films composed of oxidized organic compounds that present a condensed phase for partitioning of semi-volatile organic compounds (SVOCs), many of which are considered water-soluble. Even though “dampness” is a substantial issue in buildings, little is known about the hygroscopicity of indoor surfaces, the adsorption/absorption of water-soluble gases, the effects of liquid water on indoor surface chemistry, and the subsequent effects of that chemistry on exposure. However, even a 5 nm water film on indoor surfaces (assuming $20 \text{ m}^2/\text{m}^3$ of surface in a 300-m^3 home) will provide more than 1000 times the volume of liquid water as is found in aerosols outdoors. Since the resulting aqueous solutions will be highly concentrated, aqueous surface chemistry on authentic indoor surfaces may mimic aqueous aerosol chemistry.

We provide results to date on controlled experiments with fresh and authentic indoor surfaces—painted wallboard and window panels exposed to indoor air in real occupied homes for 4-8 months. A custom parallel plate flow reactor designed to hold indoor surface materials and a high-resolution time-of-flight chemical ionization mass spectrometer (HR-ToF-CIMS) are used to monitor uptake of acetic acid, IEPOX, ISOPOOH and hydrogen peroxide on indoor surfaces at 5%, 50% and 90% RH. The difference in RH entering and exiting the flow reactor allows quantification of water content of the indoor material at each RH. Surface film composition of glass slides from each home will be characterized by ultra-high resolution electrospray ionization QTOF-MS. This work is designed to provide quantitative constraints for indoor modeling that will ultimately improve our understanding of the impact of “dampness” on indoor exposures.

9IS.7

Modeling Water Uptake by Dust in Residential Environments. David Kormos, Karen C. Dannemiller, ANDREW MAY, *The Ohio State University*

Moisture within homes can impact microbial growth in dust, and thus, contribute to negative human health effects. However, there is currently no mathematical framework to describe this moisture uptake. To test the applicability of common atmospheric models of water uptake for the indoor environment, we conducted controlled equilibrium and kinetic experiments using Arizona Test Dust (ATD), a well-characterized model dust. In the thermodynamic experiments, ATD was incubated at equilibrium relative humidity (ERH) ranging from 50 to 100% increasing at 10% increments per day. Sample mass and water activity were recorded daily (corresponding to each ERH value). In the kinetic experiments, ATD was moved from 50% ERH to a higher level at time zero with many mass and water activity measurements performed over the course of one day in order to assess the temporal response. The kinetic experiments suggest that steady-state (equilibrium) is reached in roughly two hours.

Initial modeling efforts included the κ -Köhler equation for equilibrium experiments and the Maxwellian flux equation for kinetic experiments with constant RH. Using the literature κ value for ATD (0.025) results in an over-prediction of equilibrium water uptake, but we can infer a new value (0.0034) that matches our data well. Similarly, the kinetic equation over-predicts transient water uptake for $\kappa = 0.025$; updating to $\kappa = 0.0034$ does not remedy the issue. Consequently, we propose an alternative model that is able to capture the overall dynamic behavior, although there is still a discrepancy in the magnitude of the predicted water uptake. Regardless, both models may be able to represent indoor environments where ERH is fluctuating. Since we are ultimately interested in microbial growth (and its implications for human exposure), we couple these kinetic models with a microbial growth model for post hoc predictions of actual residential dust samples.

9IS.8

Biological Particle Resuspension from Simulated Children's Walking. Lu Zhang, Xinyue Li, Ting Zhang, MAOSHENG YAO, *Peking University*

Lower respiratory infection represents one of major killers for children below age 5 in the world. In this work, we applied a robot to simulate children's walking with shoes of different characteristics. The particle re-suspensions were simultaneously monitored by an optical particle counter and also an ATP-based bioaerosol sensor. In addition, air samples were also taken using a high volume sampler. Our preliminary results showed that walking indeed generated a significant amount of particles, and different shoes seemed to have produced different size and level particles, thus representing different inhalation exposure risks. Air samples with and without walking were being sequenced and will be presented in details during the conference. This work will further discuss how to protect children from re-suspending floor biological materials to reduce the infection risk and to protect children's health.

9IS.9

Indoor and Outdoor Levels of Traffic-Related Air Pollution and Effectiveness of Remediation Measures in a Near-Freeway School. AURELIE LAGUERRE, Pradeep Ramasubramanian, Matthew Survilo, Megan Duenas, Naveen Weerasekera, Linda George, Elliott Gall, *Portland State University*

Traffic related air pollution (TRAP) poses a threat to health and cognition, yet many buildings are located in proximity to high-traffic thoroughfares. School-age children are a susceptible population and spend a large percentage of their time inside and near schools. In this study, we investigate levels and dynamics of TRAP in a middle school located 20 – 125 m from an interstate that serves >120,000 vehicles per day. Intensive indoor and outdoor measurements are made in three phases, each consisting of ~6-weeks of monitoring. Phases consisted of i) outdoor air monitoring prior to school renovations, ii) indoor and outdoor monitoring post-renovation, following installation of remediation measures in the HVAC system and to the building envelope, and iii) indoor and outdoor monitoring six months post-renovation, following occupancy for one school year. Measurements of TRAP enable exposure assessment and evaluation of the efficacy of the renovations to reduce student exposures, including high-efficiency particle filtration and activated carbon (AC) sorbents installed in the ventilation system. Outdoor air at the school was impacted by freeway emissions, with school day-averages of black carbon, nitrogen dioxide, and ultrafine particles (UFP) of, 1490 ng/m³, 12.5 ppb, and 32700 #/cm³, respectively, with TRAP levels decreasing as function of distance away from the freeway. School day-averages of benzene, toluene, ethylbenzene and xylenes (BTEX) in outdoor air ranged 0.24 ppb to 1.10 ppb. Following renovation, comparison of upstream and downstream measurements shows filters and sorbents are generally protective for TRAP, e.g., BC removal efficiency averaged 93% while average BTEX removal efficiency ranged 63-85%, resulting in supply air pollutant levels below that of urban background. However, results show return air levels of some TRAP constituents higher than supply air, implying infiltration of TRAP is of concern in schools near freeways.

9IS.10

Ultrafine Particle Emission Interactions with Multiple Fused-Deposition Modeling (FDM) 3D Printing in Chamber Environments. Nahin Ferdousi, JOSEPH WOO, *Lafayette College*

Fused-deposition modeling (FDM) 3D printing has become extremely popular for industrial rapid prototyping, as well as for recreational and educational use. Users are commonly able to access 3D printers in shared spaces (e.g. libraries, maker spaces, and research labs) where multiple printers are placed in one centralized location. While the aerosol emissions of individual printers have been previously explored, not much is currently known about emission profiles when multiple printers and filaments are being used simultaneously in close proximity. As the formation and growth of aerosols from FDM printing is expected to depend on the gas-phase concentration of semi-volatile organic compounds emitted near print nozzle surfaces, it is expected that these concentrations will be affected by the emissions of other printers around them. Time- and size-resolved aerosol concentration profiles of two FDM printers in a controlled atmosphere chamber are presented, using varying material type (PLA, ABS, PVA), print geometry, and nozzle temperature. Aerosol emission and concentration profiles suggest that while overall emitted mass is comparable, aerosol size distributions and concentrations are different during simultaneous usage compared to the summative values of each printer used individually.

9IS.11

Surface Extractor for Deposited Indoor Aerosol. HANNAH PRZELOMSKI, Rachel O'Brien, *College of William and Mary*

Organic aerosol particles can deposit onto indoor surfaces and, once on the surface, the particles can continue to interact with the gas-phase above. Additionally, these dry deposited particles will undergo aging processes similar to processes encountered for atmospheric aerosols due to the longer timeframes for exchange indoors. These include heterogeneous oxidation, photolysis, hydration, oligomerization etc. The composition of this material is not well characterized for exposure in different indoor environments or to the different types of aging processes. A better understanding of this material is needed, including where it comes from (in terms of indoor aerosol sources) as well as how the composition varies with time. Here, a surface extractor has been designed to enable the solvent extraction of these complex mixtures off impermeable surfaces. Both aqueous and organic solvents can be used and the extractor enables good control over the solvent volume and surface area extracted. A variety of methods can be used to investigate these samples including offline-aerosol mass spectrometry as well as GC/MS and ATR-FTIR. These samples provide a complementary data set to wipe samples for indoor surfaces and enable a more complete picture of the composition and transport of indoor aerosol particles.

9IS.12

Aqueous Phase Chemistry on Indoor Surfaces. MADELINE COOKE, Andrew Ault, *University of Michigan*

Aqueous phase chemistry in aerosols and on surfaces impacts both climate and human health. Understanding these reactions is important as aqueous environments can increase rates of a reaction in comparison to the gas phase, form new species, and serve as a sink for water soluble organic and inorganic gases. Not only is there an abundance of gaseous compounds indoors capable of partitioning into the liquid phase, but there also is a greater volume of aqueous surface onto which compounds can partition due to an increase in indoor surface-area-to-volume ratios compared to outdoors. It is likely that water films on surfaces play an important role in indoor chemistry; however, there is much uncertainty in the physical and chemical properties of aqueous layers on indoor surfaces. Herein, we present a characterization of several common indoor surfaces and the associated aqueous layers under different relative humidity conditions. Physical characteristics of the water film were investigated via vibrational spectroscopic methods with a focus on the pH of the surface. To further assess the interaction of surfaces with indoor environments, aerosols of known pH were deposited onto water films of such surfaces, and the resulting change in surface pH was measured. The results of this study provide insight into potential aqueous phase reactions that could be occurring on indoor surfaces, informing predictions about the identity of indoor air pollutants and thus types of exposure to indoor occupants.

9IS.13

Dynamics of Ozone Reactivity for Different Indoor Surfaces Driven by Diurnal Ozone Exposure. MICHAEL WADE, Atila Novoselac, Richard Corsi, *The University of Texas at Austin*

Ozone reactions with indoor surfaces lead to the secondary emission of oxidized products to the indoor space. These reactions can also lead to long-term degradation of indoor materials, ranging from cultural artifacts to common indoor surfaces such as latex paint. Indoor ozone has even been reported to change the morphology of lead-based paints, increasing exposure of building occupants to lead. Previous research indicates that the reactivity of some new indoor materials with ozone decreases with exposure to realistic ozone concentrations and then regenerates during periods absent of ozone. While ozone removal to a wide range of indoor materials has been studied, the vast majority of past studies have been "one-off" (short-term) experiments that utilize new materials. In our chamber study, we tested the dynamics of ozone reactivity - driven by diurnal ozone exposure cycles of 6 hour exposure and 18 hour no exposure - for four common indoor materials: latex painted gypsum board, clay based paint, particle board, and ceiling tile. Eight samples of each material were tested for deposition velocity in experiments that simulated a five day long ozone exposure with diurnal cycles of ozone concentration. The results show that the deposition velocity varies significantly depending on material (average values ranging from 1 to 3 m/h), with the lowest value for particle board and the highest value for ceiling tile. The results also show that on a daily bases ozone reactivity is decreasing (up to 20%) for all materials. However, overnight (when surfaces are not exposed to ozone) the reactivity recovers to near the initial value from the previous day. As the surfaces were not exposed to any air overnight (no ozone exposure), the study suggests that changes in the chemical composition of material surfaces occurs during ozone cycling, perhaps due to chemical diffusion within material itself to the surface, or dynamic partitioning of lower vapor pressure reaction products between material surfaces and overlying air.

9IS.14

Are Indoor Surfaces and Aerosols Dropping Acid or Dropping the Base? Insights into Water Films and pH for Model and Authentic Indoor Samples. ANDREW AULT, Madeline Cooke, *University of Michigan*

Indoor aerosols and surfaces are complex environments that play an important role in driving gas and particle phase chemistry. These surfaces can have heterogeneous uptake, condensed phase reactions, and emitted reaction products altering the composition of indoor environments. Despite their important role, indoor aerosols and surfaces remain a mystery due to their complex and difficult to probe nature. A fundamental question that is not well understood is the acidity or basicity of indoor environments and the impact that may have on indoor gas and particle chemistry. This presentation will discuss initial results aimed at probing the properties, composition, and pH of water films on common indoor materials and model systems through systematic studies with Raman microspectroscopy, atomic force microscopy with photothermal infrared spectroscopy, and other characterization methods. These initial results offer an early glimpse into these complex systems and their role in indoor atmospheric chemistry.

9IS.15

Spatiotemporal Trends in Concentrations of Ozone and Ozone-Skin Oil Oxidation Products in an Occupied Office and HVAC System. JINGLIN JIANG, Tianren Wu, Danielle Wagner, Philip Stevens, Heinz Huber, Antonios Tasoglou, Brandon E. Boor, *Purdue University*

Ozone is an important driver of indoor oxidative reactive chemistry. Ozone can initiate the formation of indoor secondary organic aerosols through the oxidation of monoterpenes. Ozone oxidation of human skin lipids can produce volatile organic compounds (VOCs), such as 6-methyl-5-hepten-2-one (6-MHO), acetone, 4-oxopentanal (4-OPA), and decanal. HVAC systems in office buildings can deliver outdoor ozone to the indoor environment and serve as a site for heterogeneous reactions of ozone with ventilation duct surfaces and HVAC filters. The objective of this study is to explore spatiotemporal trends in the concentrations of ozone and ozone-skin oil oxidation products in an occupied office and HVAC system.

A four-month measurement campaign was performed from February-May 2019 at the Herrick Living Laboratories at Purdue University, which are four modern open-plan offices with precisely controlled HVAC systems. Time-resolved concentrations of ozone were measured with a UV photometric ozone analyzer. Ozone-skin oil oxidation products were measured via proton transfer reaction time-of-flight mass spectrometry (PTR-TOF-MS) for a portion of the campaign. An automated multi-point sampling system was built to sample ozone and volatile reaction products at eight locations throughout the HVAC system. More than ten ventilation modes with variable outdoor air exchange rates from 0 to 6 h⁻¹ were implemented, including natural ventilation via a double-skin façade.

Outdoor ozone delivered to the occupied office was found to be an important participant in indoor oxidative reactive chemistry. Prominent spatial variations in ozone concentrations were observed throughout the HVAC system. Typical ranges in ozone concentrations were: 20 to 50 ppb for outdoor air, 10 to 30 ppb for supply air, and 5 to 20 ppb for return air. Negligible ozone loss occurred across the HVAC filter bank. Indoor concentrations of ozone were found to be strongly related to the fractional amount of outdoor air supplied to the office and increased with increasing outdoor air exchange rates. Human occupants and indoor surfaces were found to be a major ozone sink in the office. Ozone concentrations decreased by ~20 to 50% from the supply to return duct, depending on the ventilation mode. Concentrations of primary (e.g. 6-MHO) and secondary (e.g. 4-OPA) ozone-squalene oxidation products exhibited diel patterns and generally correlated with carbon dioxide concentrations. 6-MHO and 4-OPA reached peak concentrations of ~0.3-0.5 ppb in mid-afternoon, with I/O ratios often exceeding 10.

9IS.16

Real Time Observations of Indoor Third Hand Smoke Emissions Transported into Non-smoking Environments via Humans. ROGER SHEU, Jenna Ditto, Christof Stöner, Thomas Klüpfel, Jonathan Williams, Drew Gentner, *Yale University*

We present the first real-time observations of indoor third hand smoke emissions from people into a non-smoking environment measured using online mass spectrometry (PTR-TOF) and also offline chemical speciation of gases and aerosols (GC-MS, LC-TOF). Despite no indoor smoking allowed at the movie theater site, we observed repeated emission events from the repartitioning of cigarette smoke tracers (e.g. 2,5-dimethylfuran, acetonitrile) into the gas-phase coinciding with the arrival of certain groups of audience members. We also observe simultaneous emissions of a wide range of aromatics, furanoids, and aldehydes, including multiple hazardous air pollutants (e.g. benzene, acrolein, styrene, and acetaldehyde), which are consistent with previously reported cigarette emissions and well-correlated with the known tracers. Concentrations of many of these volatile organic compounds are in parts per billion and increase over the course of each night and the weekend. We calculated emission rates and find that the audience experienced the equivalent of up to 5.6 cigarettes worth of secondhand smoke gases in a 1-hour period. These results demonstrate that third hand smoke is a major contributor to hazardous air pollutants and impacts indoor chemistry and secondary organic aerosol composition, especially in more confined spaces with smaller volumes and/or poorer ventilation than the theater studied here.

This study also includes the first high-resolution, non-targeted, comprehensive speciation of complex indoor aerosol mixtures without perturbation. Of the functionalized organic compounds observed via liquid chromatography, electrospray ionization in positive mode, reduced nitrogen species ($C_xH_yN_z$), mostly in the intermediate-volatility range, comprise 35% of the total abundance. Nicotine alone represents 16% of the overall abundance, and likely has an outsized impact on the indoor chemical dynamics. We observe numerous accompanying nicotine-related alkaloids and metabolites, as well as a significant amount of $C_xH_yO_zN_wS_v$ compounds.

9IS.17

Characteristics of Secondhand Marijuana Smoke: PM_{2.5} Calibration Factors and Emission Strengths. TONGKE ZHAO, Kai-Chung Cheng, Wayne Ott, Lance Wallace, Lynn M. Hildemann, *Stanford University*

The widespread legalization of recreational marijuana use has led to growing concerns about exposure to secondhand marijuana smoke (SHMS). Similar to cigarette smoke, SHMS contains particulate matter (i.e. PM_{2.5}, ultrafine particles), volatile organic compounds and carbon monoxide; in addition, it contains tetrahydrocannabinol and cannabidiol, which are well-known to cause adverse health effects. However, there are few studies characterizing SHMS.

To accurately assess PM_{2.5} concentrations in SHMS, we first focused on determining PM_{2.5} calibration factors for particles from typical types of marijuana consuming: glass pipe, joint, bong, and vaping pen. SHMS was introduced by a habitual marijuana user into a ~5 m³ chamber. To derive PM_{2.5} calibration factors, measurements from real-time optical PM_{2.5} monitors (SidePak AM510 Personal Aerosol Monitor, TSI Inc., Shoreview, MN) were compared with gravimetric mass. In addition, PM_{2.5} emission strengths for each marijuana type were calculated as µg/puff and were compared with the values for exhaled mainstream smoke from traditional cigarette smoking.

The real-time monitor's PM_{2.5} calibration factors for SHMS from a glass pipe, a joint, a bong, and a vaping pen were found to be 0.30 (SE=0.02), 0.40 (SE=0.02), 0.43 (SE=0.01), and 0.43 (SE=0.03), respectively. These calibration factors will enable more accurate real-time measurements of exposure to SHMS in field settings using portable real-time monitors.

The PM_{2.5} emission strengths of the aforementioned SHMS sources were 1.4 (SD=0.6), 4.9 (SD=0.7), 1.6 (SD=0.5), and 1.4 (SD=0.4) mg/puff, respectively. These values are ~2-6 times larger than emission strengths measured for exhaled mainstream smoke from traditional cigarettes, using the same approach (i.e. 0.8 (SD=0.5) mg/puff).

9IS.18

Heterogeneous Ozonolysis of THC and Nicotine. AARON WYLIE, Christopher Lim, Jonathan Abbatt, *University of Toronto, Canada*

Smoking is responsible for over 7 million deaths per year worldwide, with almost 1 million of these deaths caused by second-hand smoke. An additional cause for concern is third-hand smoke, which leads to exposure *via* partitioning of surface-bound smoke constituents to the immediate atmosphere after smoking has ceased. While little is known of the nature of third-hand smoke, less is known about how its constituents temporally evolve with respect to oxidation by atmospheric oxidants such as O₃ and OH. With the recent trend of recreational cannabis legalization in developed countries, understanding the nature of cannabis smoke in the indoor environment is paramount to public health. The temporal evolution of Δ⁹-tetrahydrocannabinol (THC) and nicotine, major constituents of cannabis smoke and tobacco smoke respectively, with respect to O₃ reaction on model indoor surfaces is presented. THC films of known thickness on a glass surface were exposed to clean air containing O₃ of various mixing ratios and different relative humidity (RH) values in a flowtube, and THC concentration and product formation were monitored by offline HPLC-ESIMS. The oxidation of THC followed pseudo first-order reaction kinetics independent of RH with first-order dependence on O₃ mixing ratio. Oxidized condensed-phase products were separated and putatively identified, and include secondary ozonides, epoxides and dicarbonyl products of oxidative cleavage. Product formation was heavily dependent on RH, with the presence of water favouring formation of dicarbonyl products. The surface behaviour of nicotine, both as a pure compound and within cigarette smoke extract (CSE), on glass and cotton surfaces is evaluated with respect to whether oxidation by O₃ can compete as a loss process with volatilization.

9IS.19

Characterizing Emissions from Heating Simulated Cannabis Extracts. XIAOCHEN TANG, Lucia Cancelada, Vi Rapp, Marion Russell, Marta Litter, Lara Gundel, Hugo Destailats, *Lawrence Berkeley National Laboratory*

Since the legalization of personal possession and recreational use of marijuana in California in 2016, there have been rapid increases in new ways to consume cannabis. The “Dabbing” method is growing quickly in popularity. In this practice “dabbers” place a small amount of cannabis extract on a heated surface to allow vaporization, then inhale the aerosol. This presentation focuses on understanding the composition of aerosol emitted during dabbing and its impacts on human health and indoor air quality because little information is currently available. Completely vaporizing the cannabinoids requires high temperature (as high as 400°C). Other main ingredients in the cannabis extract, such as terpenes and terpenoids, may partially decompose and form undesired harmful byproducts as gases and particles are inhaled by the user and released to indoor air. Similar emissions may be generated in smoking and vaping cannabis products.

This study assessed emissions from non-cannabinoid substances in cannabis extracts by mimicking the process of “dabbing” inside a ventilated 20-m³ laboratory chamber. Surrogate mixtures of compounds most commonly found in cannabis were prepared and vaporized on a heated surface with controlled temperature. Particle size distribution and number concentrations of the fresh aerosols were monitored with a Fast Mobility Particle Sizer (FMPS). Volatile carbonyls were collected with dinitrophenylhydrazone (DNPH)-impregnated cartridges and analyzed by liquid chromatography, while volatile organic compounds (VOCs) were sampled and analyzed by gas chromatography/mass spectrometry with thermal desorption. During the simulated dabbing large numbers of ultrafine particles were generated, as well as aldehydes and other VOCs (e.g. acrolein, methacrolein). These products are well-known irritants to the respiratory system. Therefore, heating of ingredients in cannabis extracts, and other products used as additives, may result in the formation of harmful degradation byproducts.

9IS.20

Volatilization and Partitioning of Residual Electronic Cigarette Vapor to Aerosols. HENRY COLBY, Erin Katz, Anita Avery, Peter DeCarlo, *Drexel University*

With the growing use of electronic cigarettes (E-cigs) it is necessary to understand their contribution to indoor air quality and environmental particle composition. Smoke from tobacco that deposits onto surfaces has been termed third hand smoke (THS). Like cigarette smoke, vapor from E-cigs can also collect on indoor surfaces and degrade indoor environmental quality. Chemicals in these residues such as nicotine can evaporate over time and partition to indoor aerosols which provides an additional route of exposure via inhalation. The chemicals in these residues may also be oxidized to form toxic byproducts. Laboratory experiments utilizing two different types of E-cigs were performed by introducing vapor into glass and stainless-steel chambers and allowing for particle deposition on the chamber walls. Remaining aerosols were evacuated so only the residue of the e-cig vapor remained. Ammonium sulfate aerosols introduced into the chambers and the composition of the aerosol after passing through the chamber was monitored using a high-resolution aerosol mass spectrometer (HR-AMS). 10 experiments over 7 days were performed with the glass chamber using a variety of aerosol introduction patterns. For measurements using the stainless-steel chamber, 3 experiments over 5 days were performed to investigate the change in residue composition and volatilization by monitoring the aerosol composition. These experiments provided information on how residual vapor can contribute nicotine, propylene glycol, and vegetable glycerin to indoor aerosols from evaporation and partitioning behavior. The results of these experiments will be presented showing that while residue from E-cigs can contribute chemically to indoor aerosols, the relatively simple matrix of the vapor is less chemically active than residual cigarette smoke which has been studied previously.

9IS.21

Can You Breathe Me Now? Effect of Wood Stove Exchange Programs on IAQ. MATTHEW SURVILO, Aurelie Laguerre, Everett Stilley, Elliott Gall, *Portland State University*

More than six million people in the United States use wood stoves as their primary heat source. Wood stoves emit air pollutants that may impact health, e.g., wood combustion products are associated with premature death and aggravation of pulmonary and cardiovascular conditions. Relatively little data exists reporting in-situ particulate emission rates of residential wood burning stoves. Additionally, there are few studies investigating the efficacy of wood stove exchange programs (WSEPs) as a method to improve indoor air quality (IAQ). We are partnered with a WSEP in Washington County, Oregon, to conduct an air quality study that measures the impacts of the WSEP on indoor and neighborhood levels of wood combustion products. Over twenty households are engaged in the air quality study with monitoring that employs low-cost particle counters to measure particle levels, a blower door test to approximate air exchange, and stove use monitoring. Seven households were engaged with enhanced monitoring, which added deployment of a weather station, and research grade monitors for carbon monoxide, size resolved particles from 10nm – 10 micrometers, and in select homes, NO and NO₂. All measurements occurred before and after wood stove exchange, where a newer, more efficient burning stove or gas insert was installed. Using air quality data collected simultaneously indoors and outdoors, infiltration rate estimates, and stove use data, net indoor emission rates from the woodstove will be calculated. A secondary goal of this study is to evaluate low-cost sensors (PurpleAir PA-II) for widespread monitoring of woodstove combustion. We conducted indoor and outdoor co-location with reference and gravimetric monitoring to evaluate the appropriateness of use of PA-IIs for wider scale monitoring of emissions from wood stoves. This project aims to evaluate if WSEPs have potential for improvement of neighborhood and residential IAQ in areas where wood burning is a prominent heat source.

9IS.22

Observations of Semi-volatile Siloxane Partitioning to Airborne Particles during Oven Use at Homechem. ERIN KATZ, David Lunderberg, William Nazaroff, Allen Goldstein, Peter DeCarlo, *Drexel University*

Aerosol composition measurements during a recent field campaign entitled "HOMEChem" (House Observations of Microbial and Environmental Chemistry) investigated the impact of human activities on indoor chemistry. Throughout the campaign, events simulated everyday activities such as stir frying, oven use, and bleach mopping. Numerous in-situ gas and aerosol phase instruments were deployed to analyze indoor and outdoor air during this campaign. Here, we present results from a high-resolution aerosol mass spectrometer (HR-AMS) and a thermal desorption aerosol gas chromatograph (SV-TAG). We focus on observations of high levels of siloxane mass in the particle phase during oven use at HOMEChem. Polysiloxanes, also termed silicone, consist of a linear or cyclic variable-length polymer with an $[R_2-SiO]$ monomer unit and R typically as a methyl or ethyl group. These polymers are widely used in consumer products and are also often found in building materials such as sealants and coatings. During HOMEChem oven use events, siloxane mass measured by the HR-AMS trended linearly with total aerosol mass concentration, comprising a surprisingly high 5-20% of the total. We also found that this fraction was related to the oven surface temperature. During periods when siloxane concentration was elevated, HR-AMS size distributions indicated that siloxane species matched the bulk organics size distribution characteristics. SV-TAG chromatograms acquired during oven use events provide additional insight into the types of molecules emitted and partitioned to particles; multiple lower volatility polysiloxane species were identified corresponding with oven usage. We infer that during oven use, heating of silicone/polysiloxane containing materials in and near the oven led to volatilization of these siloxane species with subsequent partitioning to indoor airborne particles.

9IS.23

An Overview of Aerosol Sources and Chemistry from the Homechem Field Campaign. ERIN KATZ, Peter DeCarlo, Atila Novoselac, Jose-Luis Jimenez, Wyatt Brown, Rachel O'Brien, Delphine K. Farmer, Marina Vance, *Drexel University*

This presentation will focus on aerosol composition measurements made by an online high-resolution aerosol mass spectrometer (HR-AMS) from a recent indoor field measurement campaign called "HOMEChem" (House Observations of Microbial and Environmental Chemistry). This study brought together a myriad of state-of-the-art analytical techniques to measure outdoor air, indoor air, and interactions between the two and with building materials. Additionally, the effect of everyday activities on indoor chemistry was investigated by performing planned perturbations to indoor air quality such as cooking, cleaning, and occupancy experiments.

We present an overview of HR-AMS data from HOMEChem beginning with baseline unoccupied periods and moving to cooking events where aerosol concentrations exceeded outdoors by ~10 times or more. In the absence of cooking activity, we find that aerosol concentrations are lower indoors than outdoors. We describe transformations of aerosols from outdoors to indoors by normalizing to the indoor-to-outdoor ratio of sulfate and find that semi-volatile partitioning from surfaces contributes additional organic mass to aerosols. We link this additional organic mass to surface samples collected during the campaign. On-line analysis of cooking aerosol during stir frying indicates that the mass spectral signature of stir fry cooking aerosol is highly correlated with the mass spectra of cooking oil, suggesting oil comprises a dominant fraction of the stir fry aerosol. We also present evidence of a source-dependent ionization efficiency for organic aerosols emitted during cooking. Finally, we describe the complex chemical composition and dynamic behavior of inorganics and organics measured in the particle phase during preparation of Thanksgiving Dinner. Notably, increases in sulfate and nitrate were observed during this event. We anticipate that the results of this study will influence how we view and control our indoor spaces to reduce exposure to indoor air pollution.

9IS.24

Indoor Particle Transformation Processes Due to Candle Burning. Su-Gwang Jeong, Lance Wallace, DONGHYUN RIM, *Pennsylvania State University*

Human exposure to indoor ultrafine particles (UFP, < 100 nm) are associated with occupant activities such as cooking and using consumer products. One of the major indoor UFP sources is candle use. Indoor UFP exposure can significantly vary with aerosol transformation processes such as coagulation, deposition and ventilation, and such processes are influenced by building operating conditions. The objective of this study is to investigate the coagulation, deposition and decay rates of indoor UFP originated from three types of candles: tapered paraffin, scented soy candles in glass jars, and beeswax pillars. In this study, particle number, surface area, and mass distributions due to candle burning for 93 particle sizes from 2 to 64 nm were examined. The relative contributions of individual particle loss mechanisms (i.e., coagulation, deposition, and ventilation loss) were characterized using the coagulation model that considered Brownian motion with the Fuchs correction along with van der Waals and viscous forces. The results show that peak number, surface area, and mass concentrations occurred at particle sizes of < 3 nm, 20 nm, and 40 nm, respectively. Relative contributions of coagulation, deposition, and air exchange rates to the total particle losses were 65.4%, 34.3%, and 0.3% at a high concentration (i.e., 106 cm⁻³), while they are 17.4%, 80.9%, and 1.7% at a lower concentration (i.e., 3 × 10⁴ cm⁻³), respectively. This result suggests that coagulation is a dominant particle loss mechanism when the total number concentration exceeds 105 cm⁻³, and it is still responsible for 20% particle loss at lower concentrations such as 4 × 10⁴ cm⁻³. These results highlight the importance of coagulation in indoor nanoparticle dynamics due to candle burning.

9IS.25

Developing a Volatility Basis Set for Indoor Cooking Aerosol Stirfry Emissions During the HOMEChem Study. MATSON A. POTHIER, Erin K. Boedicker, Jose-Luis Jimenez, Jeffrey R. Pierce, Delphine K. Farmer, *Colorado State University*

Cooking emissions are an important source of indoor aerosols and may be harmful to human health. However, the chemical composition and characteristics of these particles will impact their fate by controlling the ability of organic molecules in the particle phase to partition to the gas phase. During the HOMEChem (House Observations of Microbial and Environmental Chemistry) campaign in Austin, TX in Summer 2018, we used a thermal denuder coupled to a Time-of-Flight Aerosol Chemical Speciation Monitor (TD-ToF-ACSM). This instrument setup allows us to investigate the gas-particle partition characteristics of cooking emissions. Here we focus on cooking emissions from a frozen vegetable stir fry. The aerosol mass spectrum is dominated by organic aerosol. Positive Matrix Factorization (PMF) identified three unique factors in cooking aerosol, associated with more volatile, intermediate volatile and low volatility compounds. We probe these factors with a kinetic gas-particle partitioning model which enables us to model volatility basis set (VBS) distributions of the three PMF factors, and consider the implications of cooking emissions to indoor loadings of organic aerosol.

9NM.1

Electrically Conducting, Near Bulk Density, Micrometer Thick Metal Coatings through Room Temperature Supersonic Aerosol Deposition. YENSIL PARK, Souvik Ghosh, Christopher Hogan Jr., *University of Minnesota*

Electrical conducting coatings and thin films are commonly needed in organic solar cells and organic light emitting diodes (OLEDs) to ensure proper electrical conduction. Recent advances in additive manufacturing have led to room temperature production routes for such organic devices. However, conducting layers are typically made of metal; aside from near-room temperature liquid metals (which are expensive and often highly toxic), metal coating production requires high temperature or high vacuum techniques incompatible with most organic components. Supersonic aerosol deposition is a reduced temperature (room temperature or lower) modestly high pressure (5 Torr or higher) process where submicrometer to micrometer scale particles are passed through a converging-diverging nozzle and deposited inertially onto a substrate. Here, we demonstrate that this process can be used to produce Sn coatings from commercial Sn powder which are electrically conducting and of near bulk density. The mechanism of coating formation is the plastic deformation of particles upon impact. We show that the size distribution of the depositing powder strongly affects the deposition; simulations reveal that there is a particle size of maximum impaction velocity (near 500 m s^{-1} at 1-2 micrometers for the system utilized). Smaller particles deposit but do not appear to plastically deform, leading to poor substrate adhesion. Meanwhile, larger particles, appear to bounce from substrate and ablate away poorly adhered material.

9NM.2

Steady Uniform Production of Ultrasmall Particles via Tandem Electrostatic System for Precise Antimicrobial Activities. DAE HOON PARK, Jungho Hwang, Jeong Hoon Byeon, *Yonsei University, Korea*

Simultaneous improvement in on-demand and precise controls on material processing are critical for newly developed nanomaterials. On-demand production is receiving great interest in the realization of nanotechnologies that meet unpredictable demands of reconfiguration and modification to maximize the efficacy of materials processing. Precise control of characteristics and functionalities of materials is also receiving great interest in ensuring guaranteed efficacies and maximizing cost efficiencies. Antimicrobial nanomaterials are representatively subjects of these approaches, because they require built-to-order configurations with their stable antimicrobial efficacies for practical uses. Recent attempts to control characteristics of materials precisely have employed on-demand production systems. Consequently, developing a digitizable platform for the plug-in manufacture of ultrasmall (atomically countable) Ag or Cu particles including characteristics and antimicrobial activities of materials simultaneously was recently introduced. In this study, a tandem electrostatic system consisting of a carbon brush ionizer and a spark ablation device was developed. The spark ablation with gaseous ion injection between Ag or Cu rods was carried out to ensure the steady and uniform manufacture of ultrasmall Ag or Cu particles ($\sim 3 \text{ nm}$). The resulting particles had stronger and more stable antibacterial activities against bacteria (including multidrug-resistant strains) than Ag or Cu nanoparticles ($>10 \text{ nm}$).

9NM.3

Design of Dispersal System for Dust Detonation. SHUSIL SIGDEL, Justin Wright, Stephen Corkill, Aravind Suresh, Christopher Sorensen, *Kansas State University*

Economically and environmentally feasible methods for the treatment of contaminated grain dust, agricultural dust and waste materials of process industries are strongly preferred. Thus, we want to use particulate precursors in detonation synthesis to produce graphene. Production of graphene from toxic flour and agricultural dust will transform these waste materials into valuable materials. This work intends to design a dispersion system for a 17 L chamber to detonate the dispersed dust. We will be testing various types of dust dispersals like metal cone with mesh on top, narrow nozzle, and spiral nozzle. Performance of various type of dispersals will be shown. In addition, we can also use this dispersion system for pyrophoric metals like Mg, Al, Ti and Fe with O₂ to yield the oxides.

9NM.4

Characteristics of Graphene Produced via Detonation Synthesis. JUSTIN WRIGHT, Shusil Sigdel, Stephen Corkill, Arjun Nepal, Stefan Bossmann, Christopher Sorensen, *Kansas State University*

This paper discusses the formation of graphene via detonation synthesis. We detonate acetylene and oxygen inside a 17L chamber to form our material. By varying the ratio of oxygen to acetylene, we make graphene with different morphologies and properties. Here we explore that parameter space. We make in situ measurements of pressure and spectra using a piezocrystal and spectrometer. From these we may infer temperature and laminar flame time. We then collect the graphene from the chamber and obtain mass, density, and gaseous byproduct. From those samples we may then apply additional measurement tools such as BET, XRD, Raman, gas analysis, etc.

10AC.1

Investigation of Secondary Organic Aerosol Formation by a Filter-Based Thermal Desorption System (F-TDIS). YUANLONG HUANG, Christopher Kenseth, John Seinfeld, *California Institute of Technology*

Determination of particle-phase composition at the molecular level remains a challenge. The combination of the filter-inlet for gases and aerosol (FIGAERO), which applies thermal-driven evaporation/decomposition of particle-phase compounds, and chemical ionization mass spectrometry (CIMS) is widely used to characterize gas- and particle-phase molecular constituents. We report here the development of a filter-based thermal desorption inlet system (F-TDIS) for the CF_3O^- -CIMS, which is similar to FIGAERO but is designed for more facile filter exchange. The F-TDIS is able to reproduce FIGAERO-derived thermograms (CIMS signal vs. desorption temperature) for a wide variety of atmospherically relevant standards. The F-TDIS was applied to analysis of SOA derived from the ozonolysis of α - and β -pinene (w/, w/o OH scavenger and at different RH) in the Caltech PhotoOxidation flow Tube (CPOT). Filters for F-TDIS were collected in triplicate for each condition and treated as follows: thermal desorption by F-TDIS with ramping temperature followed by water extraction, isothermal evaporation by F-TDIS followed by water extraction, and direct extraction into water. By comparing the molecular composition of aqueous SOA extracts from filter residuals following thermal desorption or isothermal evaporation to those from "fresh" filter samples using UPLC/(-)ESI-Q-TOF-MS, together with CIMS thermograms, we evaluate the extent to which semi-volatile compounds and oligomers contribute to SOA derived from pinene ozonolysis and examine the influence of particle phase state and molecular volatility on the evolution of particle-phase composition.

10AC.2

Probing Reaction Rates in Single Aerosol Droplets Using a Branched Quadrupole Trap. GRAZIA ROVELLI, Michael Jacobs, Kevin Wilson, *Lawrence Berkeley National Laboratory*

The acceleration of chemical reactions in aerosol particles has been observed in droplets generated by electrospray ionization and characterized with mass spectrometry (ESI-MS, Yan et al. (2016)). It is still unclear what are the main contributing factors to this phenomenon (e.g. high surface-to-volume ratios in droplets, local pH inhomogeneity, surficial charge, increased reagents concentration due to rapid solvent evaporation; Lee et al. (2015)) and what is the contribution of gas-phase reactivity in ESI-MS experiments (Jacobs et al. (2019)).

Jacobs et al. (2017) developed a branched quadrupole trap where two individual charged droplets of different chemical composition (each containing one reagent) can be merged on-demand to initiate a chemical reaction. The detection of reaction products with mass spectrometry or by measuring an increase in fluorescence due to the formation of fluorescent products (or its quenching caused by the consumption of a fluorescent reagent) allows to characterize the reaction kinetics in single aerosol droplets while reliably isolating the sole aerosol condensed phase reactivity.

The aim of this work is to determine what is the role of high surface-to-volume ratios in the enhancement of reaction rates within aerosol droplets using a branched quadrupole trap. The kinetics of the reaction between o-phthalaldehyde and alanine was studied as a function of the merged droplet size (from ~ 50 μm to ~ 1 μm in radius), by measuring the increase in fluorescence signal from the composite droplet as the fluorescent isoindole product is formed.

[1] Lee, J. K., et al. (2015). *Q. Rev. Biophys.*, 48(4), 437–444.

[2] Jacobs, et al. (2017). *Anal. Chem.*, 89(22), 12511–12519.

[3] Jacobs, et al. (2019). *J. Am. Soc. Mass Spectrom.*, 30(2), 339–343.

[4] Yan, X., et al. (2016). *Angew. Chem. Int. Ed.*, 55(42), 12960–12972.

10AC.3

Influence of Evaporation Rate and Suspended Solid Concentration on Dry Particle Formation from Evaporating Aerosol Microdroplets. JUSTICE ARCHER, Florence Gregson, Daniel Hardy, Jim Walker, Rachael E.H. Miles, Jonathan P. Reid, *University of Bristol*

The evaporation of aerosol droplets containing suspensions of submicron solid particles is encountered in various engineering fields, e.g. pharmaceutical industry, bioengineering, food industry and cosmetics. Most often, the evaporation of such systems leads to the aggregation of the suspended solid particles in the droplet into a solid structure at the end of the evaporation process. Understanding what controls the final morphology of the aggregated particle is therefore a key issue for most industrial applications. The droplet evaporation kinetics during the evaporation process, as well as the morphology of the final dry solid particle structure, is highly dependent on factors such as variation in ambient temperature and relative humidity, the initial droplet composition and size, as well as the properties of the suspended submicron solid particles.

In this work, we explore how evaporative parameters (controlled atmospheric conditions – relative humidity and temperature) and the initial droplet composition (solid inclusion size and concentration) affect the droplet evaporation kinetics and the morphology of the final dry structures both during and after the evaporation process on a per-drop basis. An Electrodynamic Balance (EDB) is used for droplet kinetics measurements under tunable atmospheric conditions (265 – 325 K, 0 % to ~95 % RH) and for variable droplet parameters (droplet radius 25 - 30 μm ; inclusions-hydrophilic silica beads, 12 nm in diameter at concentrations, 0.1 – 0.5 % v/v). Additionally, a falling droplet-chain instrument is used for final dry particle collection and offline-scanning electron microscopy (SEM) imaging used for final dry particle observation. Our aim is to provide a comprehensive experimental study resulting in an improved understanding of the influence of evaporative and inclusion parameters on the evaporation kinetics and morphology of final dry products, particularly those encountered in spray-drying processes.

10AC.4

In Situ pH Measurements of Individual Microdroplets Using Aerosol Optical Tweezers to Study the Interplay between Acidity, Phase Separation, Morphology, and Reactivity. Hallie Boyer, Kyle Gorkowski, RYAN SULLIVAN, *Carnegie Mellon University*

The pH of aerosol particles controls numerous physicochemical processes and can change considerably during atmospheric aging, requiring a real-time pH micro-probe to directly study this chemistry. Highly accurate real-time pH measurements of microdroplets are obtained using our custom aerosol optical tweezers (AOT) and analysis of the Whispering Gallery Modes (WGMs) contained in the cavity-enhanced Raman spectra. Uncertainties ranging from ± 0.027 to 0.057 in pH for picoliter droplets are retrieved through averaging Raman frames acquired at 0.5 Hz over 3.3 minutes. The high accuracy in pH determination is achieved by combining two independent measurements uniquely provided by the AOT approach: the anion concentration ratio from the spontaneous Raman spectra, and the total solute concentration from the refractive index retrieved from WGM analysis of the stimulated cavity-enhanced Raman spectra. pH can be determined over a range of -0.36 to 0.76 using the aqueous sodium bisulfate system. The unique ability of this technique to directly probe pH-dependent chemical and physical changes experienced by individual microparticles such as phase separations, morphology, and heterogeneous reaction kinetics was explored using mixed organic–aqueous particles as a function of relative humidity. The interplay between heterogeneous reactions that alter pH and in turn change particle morphology that in turn feedbacks on the rate of further heterogeneous reactions and changes in pH will be presented. Aerosol optical tweezers provides a unique experimental platform to comprehensively explore the physical and chemical evolution of individual particles under long atmospherically-relevant timescales of many hours or days.

10AC.5

Electrospray Surface-enhanced Raman Spectroscopy (ES-SERS) for Studying Organic Coatings of Atmospheric Aerosol Particles. Masao Gen, Ryota Kuniyama, Atsushi Matsuki, CHAK K. CHAN, *City University of Hong Kong*

Heterogeneous reactions between atmospheric aerosol particles and gaseous pollutants, such as those forming brown carbon (BrC), represent an important mechanism. These reactions alter the particle chemical compositions and aerosol-climate interactions. While most studies assume homogeneous particle compositions, organic coatings can be formed on solid or highly viscous particles due to heterogeneous reactions but the underlying mechanism is relatively less examined. We used electrospray surface-enhanced Raman spectroscopy (ES-SERS) to directly probe the formation of BrC coatings on methylammonium sulfate, nitrate, and chloride particles from heterogeneous reactions with gas-phase glyoxal. To create BrC coatings on particle surfaces, heterogeneous reactions were performed under low relative humidity (RH) conditions (i.e. 10 or 30% RH). The reacted particles fluoresced when irradiated at 532 nm in normal Raman analysis, indirectly suggesting the presence of light-absorbing species in them. Further ES-SERS analyses showed Raman bands of 1,3-dimethylimidazole, one of the major known products of reactions of glyoxal with methylammonium, from all the reacted particles at 30% RH. However, only methylammonium sulfate particles showed the formation of BrC coatings at 10% RH. We speculate that methylammonium sulfate particles may have more surface adsorbed water (SAW) than the other particle samples to initiate the formation of BrC coatings detectable by ES-SERS. The present study highlights the surface sensitivity of ES-SERS as well as the potential importance of SAW in heterogeneous reactions of atmospheric particles with gaseous pollutants.

10AS.1

Enabling Continuous Air Quality Measurements in Cap-Haitien, Haiti – from Household Combustion to Open Burning to Political Protests. AUDREY DANG, Eben Cross, Jay R. Turner, Brent Williams, *Washington University in St. Louis*

The country of Haiti has no government air quality monitoring program, and published data are limited to less than 24 hours of continuous particulate matter measurements [1]. Thus, the potential health impacts of air quality in Haiti are poorly characterized, though prevalent solid fuel use for food cooking and open trash burning for waste disposal raise concern. In particular, over 85% of urban households in Haiti use wood or wood-derived charcoal for cooking [2]. To address this measurement gap, two ARISense nodes (Aerodyne Research) have been installed at separate locations in Cap-Haitien, Haiti since the summer of 2018. The solar-powered, mid-cost nodes integrate low-cost sensors to measure particulate matter, carbon monoxide, nitrogen oxides, ozone, and meteorological variables. We will describe these measurements and explore how political protests in Cap-Haitien during the study period have affected air quality.

[1] Davis, M.E. and Rappaport, A. (2014). *Sci. Total Environ.*, 496:22–25.

[2] Ministry of Public Health and Population, Haitian Childhood Institute, and ICF International (2018). 2016-2017 Haiti Mortality, Morbidity, and Service Utilization Survey.

10AS.2

Development of a Low-cost Air Pollution Monitoring Network in Kinshasa, Democratic Republic of the Congo. Daniel Westervelt, Anant Majumdar, R. SUBRAMANIAN, Carl Malings, Dovas Saulys, *Columbia University*

As many as 700,000 premature deaths annually are linked to air pollution in Africa, though surface measurements are scarce. Improvements in the accuracy of these estimates will require additional surface monitoring efforts, which ultimately can influence energy and emissions policy change to improve health outcomes. Over the last decade, the issue of severe air pollution has captured worldwide attention in countries such as India and China, leading to increased awareness and the beginnings of air quality improvements. However, similar focus has not occurred for most countries in Africa, including the Democratic Republic of Congo, where pollution issues are still quite severe. Kinshasa, Democratic Republic of the Congo (DRC), is a sprawling megacity of more than 11 million inhabitants in Central Africa. In March of 2018, PurpleAir sensors were calibrated and deployed at the US Embassy in Kinshasa. We present 1 year of data collected between April 2018 and April 2019 at both indoor and outdoor locations. The annual mean ambient outdoor PM_{2.5} concentration at the US Embassy Kinshasa is 48.9 $\mu\text{g m}^{-3}$, a factor of 4 above the US Environmental Protection Agency annual standard, indicating extremely poor air quality. Overall, PM_{2.5} is elevated in the months of June through October, and significantly lower in the other months. Peak concentrations occur in June through August, when rain is infrequent. Ambient outdoor daily mean concentrations can reach levels over 100 $\mu\text{g m}^{-3}$. Indoor concentrations are lower but correlate well with the outdoor ambient PM_{2.5} as expected. This project represents the first ever measurements of air pollution in Kinshasa. Future work includes further placement of sensors and measurements of gas-phase pollutants such as O₃, NO_x, and SO₂. Developing the long-term, dense urban network of air pollution monitors will provide much-needed estimates of neighborhood-scale exposures to air pollutants.

10AS.3

Low Cost, High Quality Sensors for Measuring Particle Mass and Size Distribution in a Megacity Delhi. JAI PRAKASH, Shruti Choudhry, Ramesh Raliya, Tandeep Chadha, Jiayi Fang, Pratim Biswas, *Washington University in St. Louis*

In India, one of the major hotspots of air pollution is Delhi, and its inhabitants are exposed to high PM concentrations. In order to plan for mitigation strategies, the variability of aerosol mass concentration and their size distribution are to be mapped. A newly developed low-cost and high-quality sensor by Applied Particle Technology (APT) which measures particle mass (PM_{1.0}, PM_{2.5}, and PM₁₀) and particle size distribution (0.3 μm to 10 μm) will be deployed in this study. It has customized calibration and advanced data inversion algorithms which provides accurate air quality measurements in real-time.

In the present study, APT low-cost sensor performance in the field was validated by comparison to a reference instrument (Beta attenuation monitor, BAM). The sensors are deployed at multiple locations in Delhi. After the validation of the performance, the following are the other objectives of the study: 1) temporal variation of PM_{1.0}, PM_{2.5}, and PM₁₀; 2) episodic concentration during dust storm; 3) determination of parameters that impact the size distribution characteristics of aerosols; 4) identification of local and regional sources using conditional probability function (CPF), back trajectory cluster, and potential source contribution function (PSCF). This study highlights that the low-cost sensors work effectively in the low and high polluted zones of an urban center, Delhi. The impact on urban air quality, public awareness, and policy decision makers will be presented. Results of this deployment study and the potential of the low-cost sensors will be discussed.

10AS.4

Integrating Multi-source (Satellite Retrieval, Model Simulation, Ground Based Monitoring) and Low-cost Sensor Particulate Mass Data to Improve Spatio-temporal Air Quality Mapping. CARL MALINGS, Matthias Beekmann, Daniel Westervelt, Albert A. Presto, R. Subramanian, *LISA*

The availability of low-cost particulate mass sensors is creating an opportunity for community groups, citizen scientists, and governments to assess local air quality at unprecedented spatial and temporal resolutions. More traditional high-cost, high-accuracy monitoring sites, satellite data retrievals, and chemical transport models provide additional sources of air quality data, but unfortunately no source is comprehensive on its own. Traditional monitoring networks have mainly been established for developed nations. Low-cost sensors have the potential to supplement and extend these networks worldwide but require in-field calibrations to quantify their uncertainties. Satellites provide only “snapshots” of air quality. They also require “ground-truthing” against ground-based monitors, as do computationally-intensive simulation models. Together, however, these sources of information have the potential to cover each other’s weaknesses, providing a better overall spatial and temporal picture of air quality than is available from each source independently. We demonstrate such a multi-source data integration using two case studies. In Pittsburgh, Pennsylvania, a traditional monitoring network allows for ground-truthing of satellite-based retrievals and model assimilations available from NASA’s Global Modeling and Assimilation Office. Combining this with a dense network of low-cost sensors further allows for spatial and temporal downscaling. In Kigali, Rwanda, and Kinshasa, DRC, traditional ground-based monitoring is lacking and must be substituted with low-cost sensor data. For example, a year of such data in Kigali suggests an average $PM_{2.5}$ concentration of $53 \mu\text{g}/\text{m}^3$, while the latest population-weighted average for Rwanda based on multiple data sources (Shaddick et al. 2018, available at www.stateofglobalair.org) is $43 \mu\text{g}/\text{m}^3$. Through this case study, we assess the ability of regional-scale satellite-based retrievals and local-scale low-cost sensor measurements to correct each other and yield a more accurate overall picture of air quality. Overall, we assess the potential for a multi-source approach to improve error quantification and expand spatio-temporal air quality data coverage.

10AS.5

Gas and Particle Observations from Sensor Packages Deployed in Rural Malawi and a Near-Road Monitoring Location in North Carolina. ASHLEY BITTNER, Eben Cross, Carl Malings, Eric Lipsky, Andrew Grieshop, *North Carolina State University*

Malawi, like many other Sub-Saharan African countries, is a low-income nation with a near-complete dearth of ambient air quality (AQ) observations. Reference-grade monitors have historically been cost-prohibitive in these settings, but the advent of low-cost sensor packages has created an opportunity for AQ monitoring in previously inaccessible regions. Consequently, since June 2017 we have deployed three low-cost, low-power sensor packages (Aerodyne Research Inc.’s ‘ARISense’) to three rural sites in Malawi to collect data on gases (CO_2 , CO, NO/NO₂, O₃), particles (size/count) and meteorological parameters. Before and after deployment to Malawi, the packages were collocated with regulatory monitors at a near-highway site in Durham, NC. Temperature, RH, and concentration-span data collected in NC and Malawi suggest the collocation and deployment settings are environmentally similar. Using the two collocation data sets, we compare the performance of a set of hybrid random-forest (RF), regression, and neural network calibration models to reproduce accurate concentration values and account for cross-sensitivities in the electrochemical gas sensors. We apply the calibrations to 13 months of ambient data collected in Malawi and find consistent diurnal trends (indicative of peak household cooking periods) and similar annual trends (consistent with regional agricultural-burning periods). We also compare measurements from the optical particle counter (OPC) in the sensor packages to in-situ optical nephelometer and integrated filter measurements collected using RTI’s MicroPEM devices under ambient (N = 3) and near-source conditions (N = 14). We compare the real time data to investigate the reproducibility of particle mass estimates across the two instruments and evaluate the MicroPEM response relative to varying OPC size distributions. Additionally, we examine the influence of relative humidity and other environmental factors on the OPC response. Lastly, we discuss the real-world applications and feasibility of using low-cost sensor packages in remote and challenging environments.

10BA.1

Ultraviolet Irradiation and Gaseous Iodine Treatments against Viable Bacterial and Fungal Spores Deposited on Air Filters. SERGEY A. GRINSHPUN, Worrawit Nakpan, Michael Yermakov, Reshmi Indugula, Tiina Reponen, *University of Cincinnati*

Viable bacterial and fungal spores collected on air handling filters may re-aerosolize and represent a health risk. This problem has been recognized by the bio-defense and indoor air quality communities. Methods are being developed to control stress-resistant viable microorganisms on filters. In this study, we investigated the potential of ultraviolet (UV) irradiation and gaseous iodine treatments for inactivating spores of *Bacillus thuringiensis var. kurstaki* (Btk), a surrogate of *B. anthracis*, and *Aspergillus fumigatus*, a common opportunistic pathogen used as an indicator for indoor air quality. The spores were collected on HEPA and non-HEPA filters, both flattened for testing purposes, as well as on a mixed cellulose ester (MCE) membrane filter used as a reference. A commercial HEPA unit with a deep-bed (non-flattened) filter was also tested. Combined treatments with UV and iodine on MCE filter produced a significant synergy in inactivating Btk spores. However, no similar synergy was observed for *A. fumigatus*. For spores collected on an MCE filter, the inactivation effect was about an order of magnitude greater for Btk compared to *A. fumigatus*. The filter type was found to be an important factor affecting the inactivation of Btk spores while it was not as influential for *A. fumigatus*. Overall, the combined effect of UV irradiation and gaseous iodine demonstrated some potential for inactivating spores on air handling filters. Unfortunately, the benefit of either simultaneous or sequential treatment was much lower for Btk spores embedded inside the deep-bed (non-flattened) HEPA filter as compared to the flat ones. For *A. fumigatus* the inactivation on flattened and non-flattened HEPA filters was comparable. For both species, applying UV first and gaseous iodine second produced significantly higher inactivation than when applying them simultaneously or in an opposite sequence. The data interpretation involved the spore structure and stress-response mechanisms.

10BA.2

Controlled Spore Aerosol Experiments: Radiation Exposure Dependence. Cathy S. Scotto, Matthew B. Hart, Jozsef Czege, JAY D. EVERSOLE, Steven Hill, Dan Mackowski, Jana Kesavan, Vipin Rastogi, *Naval Research Laboratory*

We provide updated results from a continuing bioaerosol radiation exposure study first described at IAC 2018. Ultraviolet photo-degradation data for aerosol particles consisting of *Bacillus anthracis*, Sterne strain spores are being obtained. Viability of total sample spores pre- and post-exposure are determined by collection onto filters, recovery into liquid, serial dilution and plating. Observed decay rates depend on the mean aerosol particle "size" (spore cluster number) due to shielding effects that have been predicted by numerical modeling.

A significant aspect of this experimental approach, is the control over which sample bioaerosol particles are generated, suspended, exposed, and collected. We have previously described our linear electrodynamic quadrupole (LEQ) trap used to confine and hold particles for long time periods.[1, 2] Concentration of the sample suspension is determined prior to the experiment, and the droplet diameters are measured by video at the capillary tip. Diameters can vary slightly from experimental run to run, but are constant during a given run, (typically about 70 μm). As the solvent component quickly evaporates, resulting residue particle "sizes" depend on spore concentration of the sample suspension.

The total number of aerosol particles for a given run also varies from run to run, typically between 300 to 500. After a sample exposure, or control, is completed, the particles are recorded as they pass through a focused laser beam on their way to a collection filter. Knowing the average number of spores per particle, and the particle number provides an accurate estimate of the total number of spores collected per run. The viable fraction is the ratio of the sample plate count to the total spore number. A significant advantage of this novel approach is that very long exposure times can be achieved with no particle loss even for relatively large particles that would normally experience gravitational settling.

[1] M. B. Hart, J. D. Eversole, et. al. Presented at the Tenth International Aerosol Conference 2018; Poster 10BA.17; American Association for Aerosol Research: St. Louis, MO, Sept. 6, 2018.

[2] M. B. Hart, et, al., Appl. Opt. 54, F174-F181 (2015).

10BA.3

Explaining the U-shaped Pattern in the Viability of Airborne Viruses vs. Relative Humidity. KAISEN LIN, Linsey Marr, *Virginia Tech*

Infectious diseases, such as lower respiratory infections and tuberculosis, are among the leading causes of death globally. Successful transmission of infectious disease requires infectious agents to remain viable during their transport from infected individuals to susceptible individuals. Thus, understanding the viability of infectious agents under different environmental conditions is critical for controlling infectious disease transmission. Our previous studies observed a U-shaped pattern in viral viability against relative humidity (RH). Specifically, the viability of viruses was higher at RH below 43% and at 100% RH, whereas it was lower at intermediate RHs. A similar pattern has been reported before but surprisingly has not been well explained yet. We hypothesized that the viability of viruses was governed by the dynamic change in solute concentrations in carrier droplets as they evaporate. In this study, we explored the evaporation of droplets at various RHs, aiming to understand the impact of RH on solute concentrations over time. We found that solute concentrations remained high at intermediate RH for an extended time, causing lethal effects on viruses. At low RHs, droplets evaporated too fast to allow solute concentrations to remain high for extended periods, and at high RHs, droplets evaporated too slowly for solute concentrations to increase significantly. In both situations, viruses were able to sustain their viability. This finding explained the observed U-shaped pattern in viability of viruses against RH, and emphasized the importance of the droplet evaporation process on the viability of infectious agents.

10BA.4

Quantifying the Relationship between Physicochemical Properties and Biological Decay in Populations of Bioaerosol Droplets. MARA OTERO-FERNANDEZ, Allen E. Haddrell, Richard Thomas, Henry Oswin, Jonathan P. Reid, *University of Bristol*

The evaporation and rehydration processes occurring during a droplet's lifetime produce rapid changes in the particles' size that will affect most of the physicochemical properties of the biological aerosol (i.e. solute concentration, density, viscosity, temperature, etc.). These dynamics could also impact the viability of the microbes contained within the bioaerosol droplets and will influence the length of time microorganisms survive during aerosol transport. To be presented is a novel approach to probe aerosols containing *Escherichia coli* MRE162 that can be extended to other microorganisms. It combines two different technologies to interconnect the complexity of aerosol dynamics with bioaerosol longevity as a function of time, environmental conditions and aerosol composition, aiming to fully understand the mechanisms of airborne transmission.

The CK-EDB (Comparative Kinetics Electrodynamic Balance) and CELEBS (Controlled Electrodynamic Levitation and Extraction of Bio-aerosol onto a Substrate) technologies are based on Electrodynamic Balance Levitation for droplet suspension and utilize droplet-on-demand aerosol generators to produce droplets with high monodisperse size distribution (Fernandez et al., 2019). By using the CK-EDB, it is possible to measure the changes in the physicochemical properties of the bio-aerosol droplets during the drying and thermodynamic equilibrium processes with the aim to ultimately interrelate this information with the biological decay responses measured by the CELEBS.

Results outlined in this presentation will contribute to understand the impact of several variables such as: (a) evaporation kinetics, (b) changes in aerosol composition, (c) presence of surfactants and (d) changes in droplet temperature on the longevity of *E. coli* in the aerosol phase, featuring some of the benefits of this novel methodology including: (1) the characterization of the first phase of microbial death during evaporation; (2) quantifying the complete droplet composition, from the single droplet to the population level; (3) minimizing stresses during bioaerosol aerosolization and sampling.

10BA.5

The Influence of Simulated Sunlight and Relative Humidity on the Inactivation of Influenza Virus in Aerosols. MICHAEL SCHUIT, Sierra Gardner, Paul Dabisch, *BNBI / DHS NBACC*

Influenza viruses are significant contributors to the global burden of infectious disease both in the United States and worldwide. Influenza transmission is believed to occur both through direct contact with contaminated fomites and by aerosol, the latter of which facilitates the rapid spread of this organism and contributes to its status as both a seasonal and pandemic public health threat. Laboratory studies with influenza virus in aerosols or liquids have generally indicated that persistence of the virus is highest at lower temperatures, in the absence of UV light, and at either low or very high humidity levels. These data support the findings of epidemiological studies demonstrating greater incidences of influenza illnesses during winter in temperate regions and little to no seasonal variability in the tropics. Sunlight is a seasonal variable known to affect the survival of many microorganisms in aerosols. However, the impact of sunlight on the survival of influenza virus in aerosols has not been previously quantified. The present study examined the survival of the PR8 strain of Influenza A virus in aerosols using an environmentally controlled rotating drum test chamber. Tests were conducted with and without simulated sunlight at both 20 and 70% relative humidity. Viral inactivation rates were quantified using a one-phase exponential decay fit to time series aerosol concentration data. Inactivation rates measured in this study were dependent on the level of simulated sunlight but were not significantly different between the two relative humidity levels tested. In darkness, the decay constant mean \pm SD was 0.001 ± 0.019 , which was not significantly different from zero ($n=10$, $p=0.85$). However, at full intensity simulated sunlight the mean decay constant was 0.252 ± 0.059 , equivalent to a half-life of approximately 3 minutes. Under these conditions, short-range aerosol transmission of the virus may be possible, but the virus would be unlikely to survive in an infectious state over long distances. These results corroborate epidemiological findings that sunlight levels are inversely correlated with influenza transmission, and can be utilized to better model influenza transmission, as well as to inform efforts to understand and limit the transmission of this virus in a variety of settings.

10CA.1

Physical Properties of Internally Mixed Soot Particles during the Carbonaceous Aerosols and Radiative Effects Study in California. Noopur Sharma, Swarup China, Janarjan Bhandari, Kyle Gorkowski, Manvendra Dubey, Rahul Zaveri, CLAUDIO MAZZOLENI, *Michigan Technological University*

Soot particles, emitted into the atmosphere during combustion of carbonaceous material, often internally mix with secondary organic aerosol. The distribution of the mixing components within each soot particle affects its optical properties and therefore the soot radiative forcing. We performed an electron microscopy analysis of particles collected in a biogenically-dominated environment in Cool, California, during the Carbonaceous Aerosols and Radiative Effects Study (CARES), in 2010. The goal was to unveil relations between different soot mixing configurations and the viscosity of the mixing organic material. Because viscous particles deform upon impact on a substrate - with the degree of deformation depending on their viscosity - we used tilted electron microscopy images to classify the organic particles into low, intermediate, and high viscosity groups based on their aspect ratio. We found that organic material in the intermediate viscosity regime almost always partially engulfed the soot particles they mixed with (90% by number). Highly viscous organic aerosol instead remained externally mixed with, or attached on the surface of, the soot particles. The viscosity of organic aerosol depends on temperature, humidity, and the material chemical composition; therefore, our findings can help model the mixing configuration of soot at given atmospheric conditions to improve the estimates of the soot impact on climate.

10CA.2

Changes of Black Carbon Sources in Beijing with Three-Year Continuous Measurements. YUE LIU, Yazhen Wu, Caiqing Yan, Tony Hansen, Mei Zheng, *Peking University*

Black carbon (BC) plays an important role in climate change, air quality and human health, especially in Beijing, China, where air pollution is still a severe problem with large population and high population density. In the past three years, BC levels in Beijing exhibit a clear decreasing trend. In this study, our objective is to examine the trend of BC in the past few years and the major sources that contribute to the reduction of BC pollution in Beijing based on 3-year continuous black carbon measurement with high-time resolution (1 min) at an urban ambient monitoring site. Information of BC measured by the 7-wavelength Aethalometer (AE-33), along with other chemical components including elemental carbon and organic carbon by a Sunset instrument, multiple metals by the Xact 625, and ions by the IGAC (in-situ Gas and Aerosol Compositions monitor) are combined to identify sources of BC. Our results show that (1) the average BC concentration was the highest in winter and the lowest in summer with a bi-modal diurnal variation in each season, (2) when comparing the dominant sources of BC between haze and non-haze periods, it was found that traffic source was the predominant source for black carbon aerosol in non-haze periods while the contribution of coal combustion and biomass burning sources increased during haze periods, (3) the three-year continuous measurements showed that the concentration of BC in Beijing significantly decreased from 2015 to 2018, (4) by comparing source apportionment results in winter from 2015 to 2018, it could be seen that Beijing has an effective control of coal combustion source especially during nighttime and it was mainly from the residential sector. However, at the same time, there is an increased importance of traffic source to BC in Beijing.

10CA.3

Influences of Primary Emission and Secondary Coating Formation on the Particle Diversity and Mixing State of Black Carbon Particles. ALEX LEE, Laura-Helena Rivellini, Chia-Li Chen, Jun Liu, Derek Price, Raghu Betha, Lynn Russell, Xiaolu Zhang, Christopher Cappa, *National University of Singapore*

The mixing state of black carbon (BC) affects its environmental fate and impacts. This work investigates particle diversity and mixing state for refractory BC (rBC) containing particles in an urban environment (Fontana, California). The chemical compositions of individual rBC-containing particles were measured by a soot-particle aerosol mass spectrometer (SP-AMS) with the single particle detection capability, from which a mixing state index and particle diversity were determined. The mixing state index varied between 26 % and 69% with the average of 48% in this study, and was slightly enhanced with the photochemical age of air masses, indicating that most of the rBC-containing particles cannot be simply explained by fully externally (0%) and internally (100%) mixed model. The average particle species diversity and the bulk population species diversity both increased with primary traffic emissions and elevated nitrate concentrations in the morning but gradually decreased with secondary organic aerosol (SOA) formation in the afternoon. Based on the single particle clustering results with the support of source apportionment of ensemble measurements, primary traffic emissions and entrainment of nitrate-containing rBC particles from the residual layer to the surface could lead to more heterogeneous aerosol compositions, whereas substantial fresh SOA formation near vehicular emissions made the rBC-containing particles more homogeneous. This work highlights the importance of considering particle diversity and mixing state for investigating the chemical evolution of rBC-containing particles. We also demonstrate that the single particle mass spectrometry technique used in this study has a great potential to improve our understanding of rBC absorption enhancement due to the presence of coating as the influences of emissions and atmospheric processes on the coating thickness and particle diversity on specific particles types and size can be better described in model simulations.

10CA.4

Long-Term Trends in Chemical Composition of PM_{2.5} in the South Coast Air Basin: A Focus on Time-integrated and Continuous Carbon Measurements. FARAZ ENAYATI AHANGAR, Sina Hasheminassab, Payam Pakbin, Andrea Polidori, Aaron Katzenstein, Jason Low, *South Coast Air Quality Management District*

Implementation of stringent regulations on stationary and mobile sources at the local, state, and federal levels over the past two decades has resulted in a substantial reduction of ambient PM_{2.5} concentrations in the South Coast Air Basin (SCAB). This study quantifies the trends in total mass and chemical constituents of ambient PM_{2.5} concentration for the period of 2004 to 2018, utilizing long-term measurements at routine monitoring stations in urban and rural areas of the SCAB. The main focus of this study is the carbonaceous species in PM_{2.5} (i.e., elemental/black and organic carbon (EC, BC, OC, respectively)).

Since diesel PM (DPM) cannot be measured directly, EC is generally used as a surrogate to estimate diesel PM. The regulatory efforts to reduce diesel emissions has resulted in significant reductions in EC emissions from the diesel fleet in the SCAB. Thus, time-integrated EC may no longer be a suitable tracer for estimating the health impacts of diesel emissions as well as assessing the relative impacts of diesel emissions and biomass burning (e.g. wildfires and residential wood combustion) on local and regional air quality and will require further investigation. This is particularly important for apportioning the impacts of short-lived air quality events such as wildfires which can fluctuate significantly across years. The light-absorbing carbon content of PM can be measured with much higher time resolution using optical methods (operationally defined as BC) and address this issue. In this study, we investigated the relationship between time-resolved BC (measured by Aethalometer AE33) and time-integrated thermal EC at different locations between 2012 and 2018. This study highlights the advantage of having high time-resolution measurements in localized air quality monitoring as well as long-term trend assessments.

10CA.5

Chemical Composition of PM_{2.5} in Zion, IL during the 2017 Lake Michigan Ozone Study (LMOS). DAGEN HUGHES, Alissia Milani, Megan Christiansen, Dylan Millet, Timothy Bertram, Charles Stanier, Elizabeth Stone, *University of Iowa*

Ambient fine particulate matter (PM_{2.5}) was collected during the Lake Michigan Ozone Study (LMOS) from May 21 to June 23, 2017 to identify the major PM_{2.5} sources affecting Zion, IL. PM_{2.5} mass concentration ranged from 1.4 – 12.9 µg/m³ and averaged 5.1 µg/m³ with elevated mass loadings coinciding with elevated ozone. The most significant contributor to PM_{2.5} mass was organic matter (OM, calculated as 1.7 x organic carbon (OC), contributing 61.8%), followed by sulfate (17.1%), ammonium (6.6%), nitrate (3.6%), and elemental carbon (EC, 3.6%). Elemental and organic tracers indicated that OM was influenced by vehicle emissions, biomass burning, and secondary organic aerosol (SOA) predominantly from isoprene. Isoprene-derived organosulfates accounted for 3.6% of OM on average, with methyltetrol sulfate being the most abundant. In comparison, organosulfates derived from monoterpenes and anthropogenic precursors accounted for 0.3% and 0.5% of OM, respectively. PM_{2.5} composition was compared between three episodes when hourly ozone exceeded 70 ppb and non-ozone periods. On June 2, ozone peaked at 91 ppb coincident with the highest PM_{2.5} mass loading and lowest OC:EC ratio (7.0), indicating a greater relative influence from combustion sources. From June 10-12, ozone peaked at 76 ppb and PM_{2.5} was heavily influenced by SOA formation as indicated by an OC:EC ratio of 17.9 and tenfold increase in methyltetrol sulfate. In contrast, isoprene SOA was relatively low from June 13-16 when ozone peaked at 88 ppb. These data demonstrate that anthropogenic and biogenic sources of PM_{2.5} organic carbon vary across periods of high ozone during LMOS. Molecular and elemental tracers will be used in positive matrix factorization to estimate PM_{2.5} source contributions to PM_{2.5}, with an emphasis on evaluating the distributions of primary/secondary and biogenic/anthropogenic sources.

10CO.1

Effect of Sodium Chloride on the Evolution of Size and Mixing State of Soot Particles from a Sooting Laminar Diffusion Flame. MOHSEN KAZEMIMANESH, Chen Kuang, Larry W. Kostiuik, Jason S. Olfert, *University of Alberta*

With global flaring volumes exceeding 140 billion m³ annually, flares are an important source of anthropogenic pollutants, such as black carbon. Hydraulic fracturing, which is a ubiquitous practice in the upstream oil and gas industry, introduces a new concern about the potential pollutants from flares as a result of flowback operations as the final stage of hydraulic fracturing. In this study, we used an open-tip sooting laminar diffusion flame, with and without sodium chloride particles introduced into the fuel flow prior to combustion, to study the effect of the latter on the evolution of size and mixing state of the particulate emissions. Methane was used as a fuel, which is a significant fraction of global flare gas. A Santoro burner was used and a 30 mm i.d. quartz tube with a length of 51 mm was placed around the fuel tube to produce a sooting laminar diffusion flame with a visible height of ~110 mm. The fuel and the overall co-flow air flow rates were 0.261 and 27.5 standard L/min, respectively. The sodium chloride concentration at the fuel outlet was ~45 ng/cm³. A 3.1 mm stainless steel tube with a 0.3 mm orifice was used to extract the sample and dilute it immediately by a factor of 1,000–12,000. The diluted sample was subsequently forwarded to a scanning mobility particle sizer and a transmission electron microscopy (TEM) sampler to study the size distributions and mixing state of particles, respectively.

The results show that in the case of the methane-only flame, the particle mode diameter increased from 56 to 77 nm with increasing HAB from 47 to 72 mm due to coagulation, although it decreased locally to ~60 nm at HAB range of 72-102 mm due to partial oxidation of soot particles near the open tip of the flame and remained constant in diameter up to height of 207 mm. In the height range of 207-437 mm, the particle mode diameter increased to ~100 nm due to further coagulation. The particle concentration in the overall HAB range decreased by two orders of magnitude from 2×10^{10} cm⁻³. In the case of methane-NaCl flame, the mode diameter increased from 39 to 45 nm in the HAB range of 47-72 mm; however, the coagulation rate was lower in this range and particles were smaller with greater concentration compared to the methane-only flame. Particles grew from 45 to 92 nm in the height range of 72-237 mm due to gradual coagulation. At HAB=287-487 mm, three modes were observed in the size distribution, with the first two modes at ~8 and 25 nm due to nucleation of NaCl particles from its vapour phase and the third mode at ~100 nm from soot particles. With further increase in HAB up to 537 mm, the size distribution became bimodal with the first mode at 25 nm and the second mode at 140 nm, while the concentration of the latter was relatively lower than that of the former. The soot particles became larger due to coagulation, either with soot or NaCl particles. The TEM images showed that until HAB of ~287 mm, the NaCl could not re-nucleate from its vapour phase due to elevated temperatures; however, at higher HABs, spherical or cubic particles of NaCl were observed mostly externally mixed and rarely internally mixed with soot particles. The size of NaCl particles from TEM images was consistent with the sizes seen in the particle size distributions.

10CO.2

On Generating Sub-100-nm Soot Particles with the Argonaut Miniature Inverted Soot Generator. JOEL CORBIN, Senaratne Amrith, Jason S. Olfert, Gregory Smallwood, Stephanie Gagne, Fengshan Liu, Prem Lobo, *National Research Council Canada*

The graphitic, strongly light-absorbing carbonaceous particles generated by incomplete combustion (soot) play a major role in air pollution toxicity and the radiative forcing of the climate. As these effects are dependent on particle size and composition, it is essential that laboratory studies are performed on soot which accurately represents real-world sources.

The Argonaut miniature inverted soot generator (MISG) employs a simple design to produce soot which is similar to real-world soot in terms of size and degree of graphitization, with a mode mobility diameter of ~150 nm achieved when using ethylene (Kazemimanesh et al., 2018) or propane (Moallemi et al., 2019) in its two-flow, air–fuel diffusion flame. These particles are useful surrogates of the soot produced by internal combustion engines or biomass combustion. However, they are substantially larger than the very small (~50 nm) and highly graphitic particles typically observed in the exhaust of aircraft engines (Vander Wal et al., 2014; Liati et al., 2014).

In this work, we therefore explore the ability of the MISG to produce aircraft engine-like soot, that is, small (<100 nm) and highly-graphitic soot. We employed a range of gas–fuel mixtures, including propane, acetylene, and oxygen-enriched air. We measured particle size using a scanning mobility particle sizer (SMPS). We evaluated the degree of graphitization by real-time measurements of the mass absorption cross-section (MAC) of our samples using the CPMA-Electrometer Reference Mass System (CERMS) and, for certain conditions, verified our interpretations using filter-based measurements of its elemental carbon (EC) content using thermal optical analysis. We found that particle size is relatively insensitive to the fuel mixture, yet certain fuel mixtures were identified which generated size distributions of approximately 100 nm mobility diameter.

10CO.3

Measuring Nanometric Carbonaceous Materials from a Sooting Ethylene Premixed Flame with the Particle Size Magnifier. FRANCESCO CARBONE, Kevin Gleason, Juha Kangasluoma, Michel Attoui, Joonas Vanhanen, Alessandro Gomez, *Yale University*

The use of the Particle Size Magnifier (PSM, Airmodus Oy.) system based on diethylene glycol (DEG) condensation growth, paved the way to the measurement of neutral and charged particles and molecular clusters in the sub 3 nm dimensional range with optical counters. The preliminary application of PSM measurements to investigate nanoparticle synthesis in metal doped flames indicated that a very high fraction of sub 3nm molecular clusters are electrically charged. Confirming such a finding in a variety of conditions would assess the role of electrostatic interactions for the nucleation of particles in flames. In this study on soot inception, the PSM system is used in an extensively studied ethylene/air premixed flame. Samples were extracted at several Heights Above the Burner (HABs) via a rapid dilution and charge conditioning system developed at Yale and were classified in terms of electrical mobility using a Half-Mini Differential Mobility Analyzer. The charge-conditioned, mono-mobile samples were treated in the PSM at different levels of DEG supersaturation, to calibrate the detection efficiency of the system for flame generated carbonaceous materials of several sizes, charge state and hydrogen content. Regardless of dilution level, results at low HABs, where soot precursor molecular clusters are small and have significant hydrogen content, demonstrate that the PSM system can detect carbonaceous materials carrying a positive (negative) charge as small than 1.2nm (1.4nm) but the detection efficiency is polarity- and composition- dependent. The detection efficiency values and its polarity dependence are both reduced at larger HABs, where the flame products lost some hydrogen. The polarity dependence of the efficiency may be related to different chemical composition of materials carrying charges of opposite polarity. This type of measurements, with a systematic assessment of PSM system efficiency to detect electrically neutral materials, will allow an accurate determination of the fraction of materials being electrically charged in flames.

10CO.4

Investigating the Distribution of Mass and Mobility Diameter of Lab-Scale, Flare-Generated Soot Using Tandem CPMA-SMPS Measurements. TIMOTHY SIPKENS, Mohsen Kazemimanesh, Melina Jefferson, Matthew Johnson, Jason S. Olfert, Steven Rogak, *University of British Columbia*

Soot contributes significantly to the anthropogenic radiative forcing responsible for climate change and to human respiratory health. The morphology of soot aggregates contributes to their impact in these roles. In response, researchers are increasingly using tandem measurements of soot mass, using devices such as the aerosol particle mass analyzer (APM) and the centrifugal particle mass analyzer (CPMA), and electromobility, using devices such as the differential mobility analyzer (DMA), to determine morphological parameters of soot. These parameters can include the effective density, shape factor, and mass-mobility exponent. However, increasingly detailed information about the soot can be obtained by considering the two-dimensional mass-mobility distribution. This requires novel approaches to deconvolving the instrument transfer functions, and the current work examines a range of candidate techniques to perform this task, including Twomey-type schemes, Tikhonov regularization, and a Bayesian approach. In this work, these approaches will be applied to soot generated from a buoyancy-driven, turbulent, lab-scale flare over a range of fuel compositions that represent real global flare gases, that is predominantly methane with varying levels of C₂-C₇ alkanes, nitrogen, and carbon dioxide. The resultant mass-mobility distributions will not only give trends in quantities like the average effective density of the particles and the shape factor as a function of fuel type but will also give an indication of how the distribution of these various quantities evolve with changes in the fuel. The results of this study can be used to develop more accurate statistical models of soot aggregate formation and their relation to the local conditions within flares.

10CO.5

Role Played by Charge in the Early Stages of Particle Formation and Growth of Titania and Soot Nanoparticles in High Temperature Flame Environment. GIRISH SHARMA, Mengda Wang, Huang Zhang, Xiaoqing You, Pratim Biswas, *Washington University in St Louis*

It is important to understand the early stages of particle formation and growth in high temperature flame environments for both nanoparticle synthesis and environmental applications. According to conventional understanding, at high flame temperatures, the particles collide with each other and coagulate to form larger particles. Contrary to this understanding, our previous work¹ shows that during the early stages of particle formation and growth (< 2 nm), charged particle fraction is very high (> 95%), suggesting that in addition to neutral particle interactions, there are charged particle, and ion-particle interactions as well.

In this work, half-mini DMA is used to study the particle formation, and growth of soot and TiO₂ nanoparticles in a premixed flame, and the role played by charge in the early stages (1 – 10 nm). Stagnation plane with hole-in-a-tube dilution probe with high dilution ratios (500-1500) is used to prevent coagulation in the sampling tube. First, positively and negatively charged blank flame ions are characterized for two different fuels (methane, and ethylene) in the presence of N₂/Ar. For studying soot inception, experiments for different flame velocities with different HABs are performed. It is found that the positively charged particle size could be as small as 1.3 nm; whereas the smallest negatively charged particle is found to be 1.0 nm. Moreover, negatively charged particles are found to be slightly smaller in size, and slightly higher in total number concentration as compared to positively charged particles. Total particle size distribution is also measured to evaluate the percentage of charged particles. On the other hand, for material synthesis early stages of titania nanoparticles formation and growth are explored for different precursor concentrations, and height above the burner. The total PSD, and charge fraction provide more insights on the role played by charge on the particle formation, and growth for both TiO₂ and soot nanoparticles starting from molecular clusters to 10 nm.

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10IS.1

Indoor New Particle Formation: An “Outsider’s” Perspective. JAMES SMITH, Michael J. Lawler, Danielle C. Draper, Sabrina Chee, Hayley Glicker, Xiaoxiao Li, *University of California, Irvine*

For the past two decades, my colleagues and I have sought to understand the species and mechanisms that are responsible for the formation and growth of atmospheric nanoparticles. Our main tool for this task has been the Thermal Desorption Chemical Ionization Mass Spectrometer (TDCIMS), an instrument developed specifically for the measurement of the molecular composition of ambient, size-selected particles as small as 5 nm in diameter. In this presentation, I will provide an overview of the insights that we have gained using TDCIMS, along with measurements performed on key gas phase precursors and other relevant parameters, focusing on the question: “What can our outdoor observations and laboratory experiments tell us about potential sources of new indoor nanoparticles?” This presentation will center on three processes that may have relevance to indoor air quality: the generation of highly oxidized compounds from the ozonolysis of organic compounds, the generation of organic and inorganic salt particles from acid-base chemistry, and the production of primary biological nanoparticles. For each of these mechanisms, I will consider the environmental conditions (e.g., temperature, relative humidity, condensation sink) and precursor concentrations that are associated with the formation and growth of nanoparticles and their relevance to indoor air quality.

10IS.2

Indoor Measurements of Nanocluster Aerosols and New Particle Formation. TIANREN WU, Philip Stevens, Heinz Huber, Antonios Tasoglou, Brandon E. Boor, *Purdue University*

A major source of atmospheric aerosol is new particle formation (NPF). NPF proceeds by the nucleation of molecular clusters as small as a single nanometer and their subsequent growth into larger sizes. Direct observations of atmospheric NPF necessitate the measurement of sub-3 nm nanocluster aerosol (NCA). While numerous studies have been conducted on atmospheric NCA, there have been no systematic investigations into NCA nucleation in occupied indoor environments. The objectives of this study are to investigate temporal trends in the concentrations and size distributions of NCA in an office and HVAC system and to characterize indoor NPF events down to ~1 nm.

A four-month measurement campaign was performed from February-May 2019 at the Herrick Living Laboratories at Purdue University, which are four open-plan offices with precisely controlled HVAC systems. NCA size distributions were measured with a nano Condensation Nucleus Counter operating in scanning mode and inverted by the expectation-maximization algorithm from the raw data. Size distributions beyond the NCA mode were measured with two scanning mobility particle sizers. Indoor and outdoor NCA was sampled from the office supply/return air ducts and outdoor air duct, respectively, using a core sampling probe. Measurements of ozone and volatile organic compounds (VOCs), via proton transfer reaction time-of-flight mass spectrometry (PTR-TOF-MS), were also conducted for a portion of the campaign.

The peeling of mandarins was found to initiate rapid indoor NPF in an occupied office. NPF was likely initiated by the ozonolysis of monoterpenes as supply air ozone concentrations were typically between 10 to 30 ppb and monoterpene concentrations often peaked at ~10 ppb during mandarin peeling. The time-scale for such indoor NPF events is much shorter than atmospheric NPF. The modal diameter of the indoor aerosol size distribution increased from 1.4 nm to 55 nm within one hour and NCA concentrations exceeded $40,000 \text{ cm}^{-3}$ at the inception of the nucleation process. During non-NPF event periods, concentrations of indoor NCA in the office were much lower than outdoors. Mean daytime and evening indoor NCA concentrations were $\sim 170 \text{ cm}^{-3}$ and $\sim 20 \text{ cm}^{-3}$, respectively. The daily maximum in indoor NCA concentrations ($\sim 270 \text{ cm}^{-3}$) appeared between 10:00 and 15:00. Measurements of outdoor NCA found a daily mean NCA concentration of $\sim 14,000 \text{ cm}^{-3}$. Frequent atmospheric NPF events were detected in the outdoor air duct of the HVAC system. NCA measurements in the office supply air duct suggest a small fraction of the outdoor NCA may penetrate the HVAC filter bank.

10IS.3

Environmental Microbes and Ambient Moisture: How Microbes Contribute to the Chemistry of Our Homes. RACHEL I. ADAMS, Sarah Haines, Katarzyna Marciniak, Karen C. Dannemiller, Allen Goldstein, Pawel Misztal, *University of California, Berkeley*

There are many potential sources of volatile chemicals in homes, and how environmental microbes contribute to this chemical milieu is not well understood. The average American house collects two pounds of dust per year; this house dust represents a large chemical and biological reservoir. We are a new research collaboration aiming to (A) develop a framework for the household conditions under which microbes are active and contribute to volatile chemistry and to (B) determine the relative importance of the composition of microbes and substrate on chemical emissions. We are using experimental systems in the laboratory to investigate the relationship between air relative humidity, household surface type, microbial inoculation, and volatile emissions. Specifically, our experiments address the following questions: (1) What are the moisture requirements for microbial growth and mVOC emissions, following the time-of-wetness model? (2) Is there an inflection point in microbial growth across increasing air relative humidity? (3) How do abiotic (substrate type and source) and biotic factors (microbial inoculation) interact to shape mVOC production? (4) Do microbes contribute to the degradation of wood into furfural and furanoid compounds under typical household conditions? (5) Can we link the gene expression of fungal communities through metatranscriptomic analysis to specific mVOCs emitted? We plan to present preliminary results from experiments conducted in the summer of 2019. This work will expand our understanding of microbially-made chemicals in indoor environments.

10IS.4

Aerosol Particles from Human Speech as a Possible Vector for Airborne Infectious Disease Transmission. SIMA ASADI, Anthony S. Wexler, Christopher Cappa, Santiago Barreda, Nicole M. Bouvier, William D. Ristenpart, *University of California, Davis*

Mechanistic hypotheses about airborne infectious disease transmission have traditionally emphasized the role of coughing and sneezing, which are dramatic expiratory events that yield both easily visible droplets and large quantities of aerosol particles too small to see by eye. Nonetheless, it has long been known that breathing and normal speech also yield large quantities of 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 particle emission during normal human speech is positively correlated with the loudness (amplitude) of vocalization, and that it varies significantly with manner of articulation and voicing. Our results indicate that certain 'phones' (the basic units of speech) associated with voiced plosives and nasals yield more aerosol particles than fricatives. We interpret these results in terms of the egressive airflow rate associated with the vocalization, which is known to vary significantly with both loudness and consonant type. Furthermore, the data reveals that a small fraction of individuals behaves as "speech superemitters," consistently releasing an order of magnitude more particles than their peers. This observation potentially explains the existence of "superspreaders" who are disproportionately responsible for outbreaks of airborne infectious disease. We use the experimental data and the Wells-Riley model to estimate the potential impact of human speech on indoor airborne disease transmission.

10IS.5

Resuspension of Particles Deposited from Consumer Nanosprays: The Effect of Surface Type, Resuspending Force, and Sampling Height. RUIKANG HE, Jie Zhang, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

Increasing application of nanotechnology has resulted in a growing number of nano-enabled consumer products. The release, deposition, and resuspension of particles from such products could be an important contributor to indoor particulate matter, with potential for adverse health effects.

This study investigated the disposition of manufactured nanoparticles from three Ag-based, three Zn-based and one Cu-based consumer sprays released indoors. Sedimentation and resuspension of released particles were investigated in a newly-constructed 2.8×1.6×2.4 m³ chamber. The resuspension of deposited particles was investigated as a function of flooring type (e.g., carpet and vinyl), resuspension force (e.g., walking by an adult and motion of a robotic sampler that simulated a child), and sampling height. Particle deposition was measured in terms of floor mass loading. Button Samplers (SKC Inc.) with 25-mm PTFE filters were used to collect sprays and resuspended particle mass at 0.3 m and 1.1 m heights, and in the experimenter's breathing zone (e.g., 1.5 m for adult and 0.3 m for simulated child). The resuspension rates were calculated for all investigated variables.

Resuspension rates ranged from 10⁻⁴ to 10⁻¹ h⁻¹, depending on the product, floor type, and sampling height. Resuspension rates were 30% to 320% higher for particles resuspended from carpet compared to vinyl, 3% to 195% higher when particles were measured at 0.3 m height than at 1.1 m height, and 19% to 243% higher when particles were resuspended by a walking adult compared to a moving robot. High particle concentrations observed at 0.3 m height showed that young children playing on the carpet could be exposed to high levels of particles resuspended by adults walking nearby.

The observed results suggest that factors affecting particle resuspension, e.g., surface roughness, walking pace, and resuspension forces due to walking should be examined closely in future studies.

11AC.1**Overview of the ACMCC Particulate Organonitrates (pON)**

Experiment. ALEXANDRE ALBINET, Jean-Eudes Petit, Andrew Lambe, Athina-Cerise Kalogridis, Liine Heikkinen, Frans Graeffe, Manuela Cirtog, Anaïs Féron, James Allan, Zainab Bibi, Tanguy Amodeo, Nicolas Karoski, Robin Aujay-Plouzeau, Laurent Meunier, Valerie Gros, Nicolas Bonnaire, Roland Sarda-Esteve, Mikael Ehn, Tuija Jokinen, Minna Aurela, Cristina Marin, Evelyn Freney, Leah Williams, Olivier Favez, et al., *INERIS, France*

Particulate organonitrates (pON) account for significant fraction of total OA in ambient air. They are formed from the reactions of volatile organic compounds (VOCs) with atmospheric oxidants (OH/NO₃ radicals) and NO_x. Their quantification can be achieved using aerosol mass spectrometry (AMS), based on the characteristic mass fragment ratio (NO₂⁺/NO⁺) allowing the distinction from inorganic nitrate. However, the accuracy of the low-resolution aerosol chemical speciation monitor (ACSM) to determine pON has not yet been evaluated. At the Aerosol Chemical Monitor Calibration Centre (ACMCC), an intercomparison for the measurements of pON has been performed in order to obtain a stable and constant generation of pON, so to compare simultaneously the response of nine different AMS/ACSM systems (long-TOF-AMS vs ACSMs; Quads vs TOFs; standard vs capture vaporizers), as well as to investigate the pON physical properties and chemical composition.

pON were generated in a Potential Aerosol Mass (PAM) oxidation flow reactor from the reaction of NO₃ radical, produced on demand (O₃ + NO₂), with single VOC precursors. Two biogenic (limonene and β -pinene) and two anthropogenic (acenaphthylene and guaiacol) pON precursors were investigated. For the determination of AMS/ACSM relative ionization efficiencies (RIE), a particle size and mass selection were achieved by combining an aerodynamic aerosol classifier (AAC) and centrifugal a particle mass analyser (CPMA). pON size distribution and total particle number concentration were monitored by a scanning mobility particle sizer (SMPS) and a condensation particle counter (CPC) allowing the characterization of the pON density. In order to get insights into the pON optical properties, as well as their chemical composition and formation processes, measurements also included cavity-enhanced absorption spectroscopy (NO₃ radical by IBB-CEAS), proton-transfer-reaction MS (PTR-MS), multi-wavelengths aethalometer (AE33), as well as filter samplings for further high-resolution MS off line analyses (GC and LC/Q-TOF-MS).

An overview of the set-up and the experiments performed will be presented together with preliminary key results.

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11AC.2**Volatility of Atmospheric Organic Nitrate Formed from Hydroxyl and Nitrate Radical Oxidation of α -Pinene and β -Pinene.** MASAYUKI TAKEUCHI, Justin Min, Rodney J. Weber, Nga Lee Ng, *Georgia Institute of Technology*

Atmospheric organic nitrate (ON) plays a crucial role in the budget and cycling of NO_x that affects ozone and secondary organic aerosol (SOA) formation. The effects of ON depend on its physical state (i.e., gas or aerosol phase) because the governing loss processes of ON could vary significantly. Further OH oxidation or photolysis for gaseous ON recycles NO_x, whereas NO_x is permanently removed from the atmosphere via hydrolysis or deposition of particulate ON. However, the physicochemical properties (e.g., volatility, solubility, etc) of atmospherically important ON are not well constrained by fundamental laboratory studies. We aim to systematically evaluate the volatility of ON formed from major biogenic volatile organic compounds via laboratory chamber experiments; the systems investigated include " α -pinene+OH+NO," " β -pinene+OH+NO," " α -pinene+NO₃," and " β -pinene+NO₃." The volatility of ON is determined by the yield-based approach using a High Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS), Scanning Mobility Particle Sizer (SMPS), and Particle-Into-Liquid Sampler coupled to Ion Chromatogram (PILS-IC), and by the thermogram-based approach using a Filter Inlet for Gases and AEROSols coupled to a High Resolution Time-of-Flight Iodide Chemical Ionization Mass Spectrometer (FIGAERO-HR-ToF-I-CIMS). Two methods are generally in a good agreement, though the yield-based method tends to measure a larger contribution of semi-volatile species than the thermogram-based approach. ON is found to be generally less volatile than previously measured for " α -pinene+OH+NO" and " β -pinene+NO₃" systems. The discrepancy appears to stem from the limited range of organic mass loading conditions explored in past studies. Moreover, there are some fractions of low-volatility ON compounds that are essentially non-volatile in atmospherically relevant conditions ($C^* < 0.1 \mu\text{g m}^{-3}$); such low-volatility ON has not been reported in previous studies. Our estimated volatility values serve as the experimental constraints for parameterization of monoterpene ON in models, facilitating more accurate predictions regarding the role of ON in ozone and SOA formation.

11AC.3

Organic Nitrate and Secondary Organic Aerosol Formation from the Reaction of Alpha-Pinene and Nitrate Radical under Simulated Ambient Conditions. GUY BURKE, Yichen Li, Tran Nguyen, *UC Davis*

The atmospheric chemistry of the nitrate radical (NO_3) with monoterpenes is important in understanding ozone and secondary organic aerosol (SOA) formation in the Southeast United States and other regions of mixed biogenic and anthropogenic influence. This chemistry produces NO_x reservoir species like organic nitrates (ON) and may be an important source of SOA. However, our knowledge of the NO_3 reaction with the most abundant monoterpene, alpha-pinene, has significant uncertainty. Previous studies reported a large range in the SOA and ON yields from the alpha-pinene + NO_3 oxidation and did not capture some of the key chemical species observed in the field. This is likely due to the different experimental conditions and the challenge of capturing ambient nighttime and night-to-day transitional chemistry in chamber studies. We studied the alpha-pinene + NO_3 reaction in an atmospheric chamber, with particular focus on the RO_2+HO_2 channel, which resulted in the formation of the nitrooxy hydroperoxides and other ON species that are observed at the SOAS 2013 Campaign, and reduction in the RO_2-RO_2 and $\text{RO}_2 + \text{NO}_3$ reactions that are not expected to be important in the ambient environment. The yields of gas phase products are measured with CF_3O^+ chemical ionization mass spectrometry (CIMS) and the SOA composition is analyzed with liquid chromatography high-resolution mass spectrometry (LC-HRMS). We will discuss the dependence of ON and SOA yields with respect to reaction conditions such as the estimated concentrations of NO_3 and HO_2 .

11AC.4

Experimental Investigation of the Gas- and Particle-Phase Products and Mechanism of Reaction of Δ -3-Carene with NO_3 Radicals. MARLA DEVAULT, Paul Ziemann, *University of Colorado*

Oxidation products of monoterpenes have been shown to contribute to SOA formation in the atmosphere. However, the nighttime oxidative processes, which are dominated by nitrate (NO_3) radical addition to alkenes, are not well understood. In order to fill this gap, we have quantified the yields of gas- and particle-phase products of the nitrate radical-initiated oxidation of Δ -3-carene, a monoterpene that is primarily released by coniferous plants. Based on these yields, we have developed a reaction mechanism and calculated branching ratios for key reaction pathways. Experiments were conducted at ambient temperature and pressure at 55% RH in a dark 8 m^3 Teflon chamber using N_2O_5 to generate NO_3 radicals via thermal decomposition. The initial monoterpene: N_2O_5 ratio was 3:1, deliquesced ammonium sulfate seed particles were used, and the aerosol was monitored online using an Electron Ionization Thermal Desorption Mass Spectrometer and a Scanning Mobility Particle Sizer. After reaction completion, SOA was collected onto a Teflon filter and extracted for analysis. The bulk functional group composition was determined using a set of derivatization-spectrophotometric analysis techniques and Fourier-Transform Infrared Spectroscopy. Products containing nitrate groups (comprising most of the SOA) were separated and quantified using HPLC-UV-Vis and identified using an Electrospray Ionization Mass Spectrometer, Chemical Ionization Ion-Trap Mass Spectrometer, and Electron Ionization Mass Spectrometer. Gas-phase products were collected onto an annular denuder coated with a derivatizing agent for carbonyl groups, extracted, and analyzed by the same methods. Altogether, the mechanism derived from the measured gas- and particle-phase product yields will inform regional and global models on the contribution of nighttime oxidation of monoterpenes to SOA.

11AC.5

A Laboratory and Modeling Investigation on the Effects of Amine Uptake on SOA Composition and Its Potential Impacts on Air Quality. JULIA MONTOYA-AGUILERA, Natalie Smith, Shupeng Zhu, Donald Dabdub, Sergey Nizkorodov, *University of California, Irvine*

Inorganic nitrogen contributes significantly to particulate matter (PM) and is represented 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. Reactive uptake of reduced nitrogen compounds by SOA, specifically ammonia (NH₃) and amines, leading to the formation of NOC remains unaccounted for in air quality models. Atmospheric NH₃ is ubiquitous and expected to rise due to intensifying use of NH₃-based fertilizers. This uptake is important to characterize because of its potential effects on SOA composition and ability to reduce NH₃ contribution to inorganic PM formation.

Uptake of NH₃ and dimethyl amine (DMA) by SOA was investigated in this study. Anthropogenic (toluene, n-hexadecane) and biogenic (limonene, cedrene) volatile organic compounds were oxidized in a smog chamber at various relative humidities (0-50%). After initial SOA formation, a pulse of NH₃ or DMA was introduced into the chamber. Mass spectrometry was used to characterize chemical composition in the gas phase (proton-transfer-reaction time-of-flight mass spectrometer) and particle phase (time-of-flight aerosol mass spectrometer). An NH₃ analyzer measured NH₃ or DMA decay. The kinetics of the NH₃+SOA→NOC reactions depended on the SOA system, with measured uptake coefficients of 10⁻⁵ to 10⁻³. Overall, DMA uptake was greater than NH₃ uptake by toluene, limonene, and cedrene SOA. The Community Multiscale Air Quality Modeling System with a continental U.S. domain indicated that inclusion of NH₃+SOA→NOC chemistry decreases the concentration of inorganic components of PM_{2.5} but increases biogenic SOA, especially in the southeastern U.S.

While some of the NH₃ uptake by SOA results were published in 2018, the DMA results are new and will be presented at AAAR for the first time.

11AC.6

Observed Particle Phase Chemistry Deviates from Brown Carbon Formation in Bulk Solutions. HENSLEY JACK, Adam Birdsall, Valtierra Gregory, Frank Keutsch, *Harvard University*

Condensed-phase reactions involving carbonyls and amines have been shown to produce light-absorbing heterocycles that could affect aerosol radiative forcing. The proposed chemistry in aerosol particles is typically extrapolated from studies that characterize chemical reactions in bulk solutions. The underlying assumption is that the aerosol particle and a bulk solution serve as similar reaction media, but in reality, chemical mechanisms could differ in these two systems. Here, we study the reaction of butenedial (C₄H₄O₂) and ammonia, and juxtapose their reaction in bulk solutions (~1-10 mL) with reaction in aerosol particles (~10 micron radius). We use NMR spectroscopy to characterize the formation of pyrrolinone (C₄H₅NO) in capped bulk solutions containing butenedial and ammonium sulfate, which darken as the reaction proceeds. To examine this chemistry over comparable timescales in actual aerosol, we apply a newly developed instrument: single particle levitation with an electrodynamic balance coupled to mass spectrometry (EDB-MS). We employ the EDB-MS technique to demonstrate that pyrrolinone formation in butenedial / ammonium sulfate particles is inhibited unless significant ammonia is fed into the surrounding gas phase. By contrast, in the capped bulk system, ammonia and reaction intermediates are not depleted from the condensed phase as they partition to the surrounding gas phase. This work illuminates the role of gas-particle partitioning as a critical control on reaction progress in aerosols, where surface area-to-volume ratios are large with respect to bulk solutions.

11AS.1

Estimating Personal Exposures from a Multi-Hazard Sensor Network. KIRSTEN KOEHLER, Christopher Zuidema, Larissa Stebounova, Sinan Sousan, Alyson Gray, Oliver Stroh, Geb Thomas, Thomas Peters, *Johns Hopkins Bloomberg School of Public Health*

Occupational exposure assessment is almost exclusively accomplished with personal sampling. However, personal sampling can be burdensome and suffers from low sample sizes, resulting in inadequately characterized workplace exposures. Sensor networks offer the opportunity to measure occupational hazards with a high degree of spatiotemporal resolution. Here, we demonstrate an approach to estimate personal exposure using hazard data from a sensor network. We developed a multi-hazard monitor, constructed with low-cost sensors for particulate matter (PM), carbon monoxide (CO), oxidizing gases (OX) and noise (using a sensor developed in-house), and deployed a 40-node network in a heavy-vehicle manufacturing facility. During typical production periods, one-hr mean hazard levels \pm standard deviation across all monitors for PM, CO, OX and noise were 0.62 ± 0.2 mg/m³, 7 ± 2 ppm, 155 ± 58 ppb, and 82 ± 1 dBA respectively. Next, we simulated stationary and mobile employees that work at the study site. Network-derived exposure estimates compared favorably to measurements taken with a suite of reference direct-reading instruments deployed to mimic personal sampling but varied by hazard and type of employee. The RMSE between network-derived exposure estimates and reference measurements for mobile employees was 0.15 mg/m³, 1 ppm, 27 ppb, and 3 dBA for PM, CO, O₃ and noise, respectively. Pearson correlation varied by hazard in the combined time periods of the mobile routines, it was highest for CO ($r = 0.66$) and lowest for noise ($r = 0.39$). Correlation between network-derived exposure estimates and reference measurements ranged from 0.39 (noise for mobile employees) to 0.75 (noise for stationary employees). Despite the error observed, the use of sensor networks to estimate personal exposures easily, frequently, and on many people holds promise as a way to complement sparse data obtained with traditional personal sampling.

11AS.2

Big Data and Air Quality: Using Twitter Data for Air Quality Monitoring. Supraja Gurajala, SURESH DHANIYALA, *SUNY Potsdam, NY*

Low-cost sensors are increasingly being deployed to widen our air quality monitoring network. Such sensors have conventionally been physical sensors, but here we explore the possibility of using social media data for air quality sensing. Such sensing would be low-cost but not necessarily low in complexity or value. Social media posts represent a real-time public response to a wide range of events, including air quality. Several studies have shown that the number of posts on Weibo, a Chinese social media site, were closely related to air quality levels at corresponding locations in China. Social media data based analysis may allow us to understand the quality of air at locations where monitoring is absent or in locations where air is monitored, social media analysis might allow us to understand public response to air quality. Here, we investigate the ability to use Twitter data to predict air quality and understand public response to air quality events. Accurate model generation first requires identification of an appropriate subset of tweets best related to air quality levels. Using air quality-related tweets for over a duration of year and a bag-of-words representation of tweets, we generated a machine learning based model to predict air quality in different locations around the world. The ability of the generated social media model to predict air quality at locations and time periods different from those used for calibration was then evaluated. We will present our model generation approach and report on the ability the social media models to be used for global predictions. Additionally, we will also discuss how these social media models can provide information about public's response to air quality that is difficult to obtain otherwise.

11AS.3

Spatiotemporal Modeling of PM_{2.5}, CO and NO₂ Concentrations Measured by a Low-cost Sensor Network: Comparison of Linear and Machine-learning Enabled Land Use Models. SAKSHI JAIN, Albert Presto, Naomi Zimmerman, *University of British Columbia*

Many previous studies have characterized spatial patterns of pollution by building land use regression (LUR) models from distributed passive samplers or filter samplers. These models can be generated with high spatial resolution, thereby producing estimates of long-term (e.g., annual average) spatial patterns in concentration, but generally have poor temporal resolution. Deployment of low-cost sensors, which typically sample in real time, creates the possibility of time-resolved and/or real-time modeling of concentration surfaces.

The aim of this study was to develop spatiotemporal models for PM_{2.5}, CO and NO₂ using measurements collected by a network of low-cost sensors in Pittsburgh, Pennsylvania. Models were developed for daily average concentrations for periods spanning August 2016 – December 2017 across 50 unique sites. Land use variables included 15 different time-independent (e.g., elevation) and time-dependent (e.g., temperature) predictor variables. We examined two different models: LUR and a machine learning enabled land use model (land use random forest – LURF) that uses random forests to link observed concentrations to land use variables. A hybrid LUR-LURF model was generated to resolve the shortcomings associated with individual models. The models were also evaluated using time-decomposed signals (e.g., short-lived spikes vs. long-term enhancements).

Time decomposition of signals resulted in equal (PM_{2.5}, CO) or better (NO₂) R² values, especially for LUR models. LURF models outperformed LUR models in all cases. PM_{2.5} LURF and hybrid models were characterized by high R² (median~0.7), low normalized mean absolute error (CvMAE, median~ 20%), and low variability. NO₂ time-decomposed models had higher R² (~20% improvement), slightly lower CvMAE values (~10%), and lower variability as compared to their standard signal counterparts. The results of our study show that a combination of low-cost sensors and novel data analytics can be successfully used to build more robust land use models, locate hotspots and provide preliminary information about air pollution gradients to policymakers.

11AS.4

Integrating Low-cost Sensor Networks with Fixed and Satellite Monitoring Systems for Enhanced Accuracy, Reliability, and Applicability. JIAYU LI, Huang Zhang, Chun-Ying Chao, Chih-Hsiang Chien, Chang Yu Wu, Cyuan-Heng Luo, Ling-Jyh Chen, Pratim Biswas, *Washington University in St Louis*

A reliable data source for air quality communication, pollution mapping, and exposure estimation is particulate matter (PM) mass concentrations measured in conventional monitoring stations. A high spatiotemporal density of monitoring stations is essential to achieve a better understanding of PM transport on a regional and global scale and to accurately establish the impacts of such PM, for example, health effects. However, due to the cost and operational complexities, a limited number of such real-time PM monitors can be deployed. PM mass concentration can also be retrieved from aerosol optical depth (AOD) data collected by remote sensing, but these datasets are usually compromised by weather conditions and aerosol optical properties. Monitoring station networks are normally located in populated areas, while remote sensing can cover sparsely populated areas. To increase the measurement density, a network of low-cost PM sensors is a promising approach. With the advent of low-cost PM sensors and advances in data analytics, we have proposed integration of information from multiple measurement approaches. In this study, we demonstrate this approach by synergizing the data from 75 monitoring stations, 2,363 AirBox low-cost sensors, together with Terra remote sensing data for the main island of Taiwan. A machine learning method is utilized to select the useful data from the massive AirBox datasets. Ordinary kriging is used to create a visual PM distribution map. The AirBox and remote sensing datasets are calibrated with data from collocated monitoring stations. The maps created from these three data sources demonstrate an approximate 30-fold synergistic improvement in the spatial resolution of PM mapping, with minimal bias. This method will greatly assist the validation of PM transport models and enhance the accuracy of exposure estimations. With this method, we identified a special pollution event during a Typhoon approached Taiwan.

11AS.5

Improving the Performance of Low-Cost Optical Particle Counters with Machine Learning: Applications for Indoor Aerosol Measurements. Satya Sundar Patra, RISHABH RAMSISARIA, Ruihang Du, Tianren Wu, Brandon E. Boor, *Purdue University*

Machine learning-based calibration techniques are emerging as a viable option to improve the field performance of low-cost optical particle counters (OPCs). Raw particle number and mass concentration data provided by low-cost OPCs is often inaccurate and subject to uncertainties. The objective of this study is to apply machine learning techniques to improve the accuracy of low-cost OPCs in measuring accumulation and coarse mode aerosols in residential buildings.

A two-month field campaign was conducted from November 2018-January 2019 at the Purdue ReNEWW (Retrofitted Net-zero Energy, Water, and Waste) House to collect training and testing data for low-cost OPCs. Three adult residents occupied the house throughout the campaign. The OPCs report raw particle counts across sixteen size fractions from 380 to 17,000 nm in optical equivalent diameter. The OPCs were integrated with Raspberry Pi running a custom Python script. Co-located training aerosol instrumentation included a scanning mobility particle sizer (SMPS: 10 to 380 nm) with a long differential mobility analyzer and an optical particle sizer (OPS: 380 to 10,000 nm). The field campaign included a one-week training period and a seven-week testing period. Throughout both periods, the OPCs sampled aerosols of indoor and outdoor origin with variable optical and morphological properties.

The machine learning-based field calibration method was implemented during the one-week training period and included two stages. First, support-vector machine and gaussian process regression models were applied to correct the size-resolved counting efficiency of the OPCs from 380 to 10,000 nm using the OPS as the reference. Then, another gaussian process regression model was used to predict the number, volume, and mass of indoor aerosols below the 380 nm detection limit of the OPCs, using the SMPS as the reference. The machine learning correction approach reduced the mean absolute percentage error for OPC-based size-integrated particle number, volume, and mass concentrations (100 to 2,500 nm) from > 80% to within 10% compared to the training instrumentation during the seven-week testing period.

11AS.6

Community-owned Air Quality Monitoring in East Boston, MA: An Integrated Approach to Air Health. SCOTT HERSEY, Eben Cross, David Hagan, Jared Briskman, Lacie Fradet, Lauren Gulland, Isabel Harrison, Jonathan Jacobs, Linnea Laux, Samuel Myers, Louise Nielsen, Taylor Sheneman, Katerina Soltan, Jonah Spear, *Franklin W. Olin College of Engineering*

A unique academic-industry-nonprofit partnership was formed in 2018 for the purpose of creating a culture of air health in East Boston, Massachusetts - immediately adjacent to Boston's Logan Airport. Using a human-centered and interdisciplinary approach, collaborators from Olin College of Engineering, Aerodyne Research, Inc., and Airport Impact Relief, Inc. (AIRInc) engaged in three project components to achieve community-identified objectives. First, the team established a network of 8 ARISense nodes measuring CO, NOx, O3, CO2, and size-resolved particle concentrations larger than 300 nm, with locations chosen to capture impacts from ascending and descending aircraft, ground-based airport operations, and on-road emissions. A van with reference instrumentation provides continuous, collocated validation and improvement of calibration approaches. A custom software ecosystem was built to apply machine learning calibration algorithms and ongoing calibration evaluation before sending data to a database that is integrated with a frontend with separate UX for citizens and researchers. With this software, residents are able to evaluate hyper-local air quality at 1 minute resolution in order to visualize otherwise invisible pollutants and make decisions about outdoor activity to reduce exposure. Next, the team established an awareness to agency campaign focused on coupling raised awareness about degraded air quality around the airport with scientifically sound information about health impacts and sources of pollutants in the area, as well as low-barrier-to-entry opportunities to take personal action to reduce exposure. Finally, having demonstrated the efficacy of in-home HEPA filters at reducing exposure in the East Boston context, collaborators ran a pilot subsidy program aimed at improving access to filters. Here, we describe the components of this community-centric approach and present data from the network of ARISense nodes along with an exploration of uncertainties and limitations via comparison with the collocated reference station.

11BA.1

Characterization of M. Tuberculosis Lipids in Exhaled TB Bio-aerosols. Robin Wood, Dapeng Chen, Wayne Bryden, CHARLES CALL, *Desmond Tutu HIV Research Centre, University of Cape Town*

Introduction

Tuberculosis (TB) transmission requires expulsion of viable bacteria in respirable aerosols from infected individuals. Detection of infectious individuals depends on exhaled air volume sampled, efficient capture of respirable particles generated from infection sites and sensitive identification of bacterial markers.

Methods

Newly diagnosed TB patients remained in a compact personalised clean room for 60 minutes. Airborne particles were collected into liquid using a high flow (300 lpm) cyclone (Coriolis- μ Bertin™), sampling approximately 500 liters of exhaled air. Centrifuged pellets of collected fluid were stained with a novel salvatochromic trehalose probe to identify viable organisms and supernatant was used as substrate for *Mycobacterium tuberculosis* lipid mass spectrometry (MS) analysis. Lipids were extracted using Folch method and high resolution MS performed with Orbitrap 120,000 mass resolution mass spectrometer (FWHM) in positive and negative ion modes. Signal to noise ratios > 5 and MS/MS analysis enabled accurate mass measurements and identification of unique TB cell wall-associated lipids.

Results

For positive ion mode, 3 control, 19 TB, and 14 non-TB samples were included. Principal component analysis distinguished between non-TB and TB samples. However, 4 TB samples were overlapped with non-TB samples. In addition, in positive ion mode, non-TB patients showed small in-group difference while TB samples showed larger in-group differences. For negative ion mode, 3 control, 18 TB, and 17 non-TB samples were included. PCA distinguished non-TB and TB samples but 3 TB samples were over-lapped with non-TB samples. Non-TB and TB showed in-group differences.

Conclusions

High-volume liquid cyclone sampling with novel viability staining and mass spectrometry analysis, identified live mycobacteria and specific mycobacterial lipids in TB patient derived bio-aerosols. Characterization of peripheral lung-derived bio-aerosols reflect novel surrogate markers of TB disease.

11BA.2

Aerosolization-Based Techniques to Synthesize Pulmonary Drug Carrier Microparticles for Tuberculosis Therapy. CHETHANI ATHUKORALA, Hema Ravindran, Shantanu Sur, Suresh Dhaniyala, *Clarkson University*

Tuberculosis (TB) bacilli often reside inside macrophages and stay protected by intracellular localization, leading to an inefficient response to antitubercular drugs delivered through conventional methods. Inhalational delivery of anti-TB drugs is gaining interest for its potential to deliver the drug efficiently into the affected lung regions. The objective of our study is to design a core-shell micro particle for antitubercular therapy deliverable via respiratory route and capable to target lung macrophages. The biopolymer alginate core will enable a sustained release of anti-TB drug; the shell consists of self-assembled peptide nanofibers will provide macrophage targeting through presentation of macrophage-specific tuftsin epitope. For an efficient delivery of drug in the deep lung tissue, we have developed aerosolization based-techniques to generate alginate particles in the size-range of 500 nm to 3 μ m. Atomization was combined with various collection techniques such as impinging, gravity settling, and charge based electrostatic collection to find the optimal method for our purpose. We noticed that the mean size of collected alginate particles was dependent on the technique used. These techniques were compared with well-known particle collection methods, such as SKC BioSampler and Anderson Impactor. The interaction of these tuftsin epitope presenting core-shell microparticles with macrophages is currently being investigated in an in vitro model. As a long-term objective, the generated microparticles will be tested to study their deposition dynamics in airway system using modelling and mice lung tissue distribution.

11BA.3

Improved Discrimination Between Dust and Bioaerosol by Aerosol Time-of-Flight Mass Spectrometry. GAVIN CORNWELL, Camille Sultana, Markus Petters, Hashim Al-Mashat, Nicholas Rothfuss, Hans Taylor, Paul DeMott, Sonia Kreidenweis, Andrew Martin, Kimberly Prather, *University of California, San Diego*

Ice nucleating particles (INPs) are rare atmospheric particles that can greatly affect clouds and precipitation through their ability to trigger cloud glaciation at warmer temperatures than would occur in their absence. Two particle sources that have been shown to be particularly efficient at initiating ice formation in clouds are dust and bioaerosols. Dust has modest ice nucleation (IN) activity at temperatures below $-15\text{ }^{\circ}\text{C}$ and is emitted and transported at high altitudes globally in significant quantities. Bioaerosols are less abundant, but certain species possess exceptional IN-activity and may be especially important due to their ability to trigger ice formation at temperatures as warm as -1°C . Single particle mass spectrometry is a sophisticated but technically challenging method for in-situ measurements of INP composition. Of particular concern is that dust and bioparticles have overlapping mass spectral features, complicating their unambiguous detection. In this work, we present a detailed analysis of standards for dust and bioaerosol. Using insights informed by this analysis, we developed a decision tree for the identification of cellular bioaerosol at a site in coastal California using an aerosol time-of-flight mass spectrometer. These particles showed moderate correlations with a subset of fluorescent particles measured by the wideband integrated bioaerosol sensor and displayed temporal profiles that tracked INP concentrations measured at $T = -15\text{ }^{\circ}\text{C}$, suggesting that this particle type could serve as a useful proxy for INPs active at modest supercooling.

11BA.4

Modelling the Transport of Infectious Aerosols in Containment Patient Care Settings Using DNA-tagged Microspheres. JOSHUA SANTARPIA, Danielle Rivera, Kevin Crown, Sean Kinahan, John Lowe, Jocelyn Herstein, *University of Nebraska Medical Center*

The West African Ebola outbreak from 2014-2016 brought the care of patients with highly infectious diseases into the public concern. The infection of a caregiver in a U.S. hospital highlighted the need to care for these patients in specialized facilities. Ongoing outbreaks of Ebola, and increasing concern over highly infectious diseases that can be transmitted via the respiratory route (coronaviruses, influenza, etc.) highlight the need to understand the behavior of potentially infectious aerosols in a patient care environments designed for containment of these diseases. Since it is both unsafe and impractical to use infectious particles to examine the spread of particles in these environments, particularly in active hospital and patient care environments, new methods are needed. In this study, DNA-tagged microspheres of known size are used to examine particle dispersion in the Biocontainment Unit of the University of Nebraska Medical Center, where several Ebola patients were cared for during the 2016 outbreak and in a model, portable containment patient care unit. In the latter, mock patient care was performed by trained technicians to demonstrate how patient care activities may spread aerosolized particles. Findings indicate locations where air sampling may be beneficial to determine the aerosol hazard of a new infectious disease, if it is unknown, and demonstrate the degree to which an infectious aerosol may be transported by patient care activities.

11BA.5

Exhaled Breath Aerosol Collection Methods. CHARLES CALL, Wayne Bryden, Dapeng Chen, Robin Wood, *Zeteo Tech*

Tuberculosis (TB) is one of the oldest recognized diseases in human history and has resulted in the deaths of as many as one billion people over the course of time. Currently the World Health Organization estimates that 1/3 of the world's population has a latent case of tuberculosis. From this pool of roughly two billion people, over 10 million active cases arise each year. It is the leading cause of death by infectious disease worldwide and it is known to be transmitted by exhaled breath. Viral infections are a constant threat to the global population. Coronaviruses such as that which causes Middle East Respiratory Syndrome (MERS) are also believed to be spread by exhaled breath aerosol.

Our research team is investigating mass spectrometry-based methods to assess disease status in tuberculosis patients. In the future, we anticipate screening populations in high-burden settings to identify previously unknown cases of tuberculosis and assess a patient's infectiousness to others. The focus of our breath aerosol collection research activity is to assess the effectiveness and optimization of exhaled breath aerosol (EBA) collection methods.

Aerosol collections were completed using three healthy volunteers. Exhaled breath was sampled using a pre-determined set of deep breathing protocols. Several aerosol collection technologies were used, including a wet-walled cyclone and two types of filters. Filter samples were analyzed by mass spectrometry to semi-quantitatively compare the collection methods and respiratory protocols by quantifying signal to noise ratios for specific lipids present in the aerosol samples.

Collection of breath aerosol is challenging due to the constant variability and large range in flow rate during normal or prescribed breathing protocols, and due to the dynamic size distributions of the aerosol due to changes in humidity and temperature as the aerosol enters the ambient environment. This presentation will present results that compare the aerosol collection technologies for a given respiratory protocol and will assess the effectiveness of each breathing protocol to generate EBA. Specific challenges associated with quantitation of each EBA collection method will be reviewed.

11BA.6

Non-invasive Measurement of Viral Load in Distal-Airway Lining Fluid through Characterization and Collection of Exhaled Breath Aerosols. SOMAYEH YOUSSEFI, Jennifer German, Donald Milton, *University of Maryland School of Public Health*

Infectious fine particle aerosols are generated from the human lung during influenza and other acute respiratory infections (ARIs) and may play an important role in transmission. These aerosols are generated from closure and reopening of small airways and shear forces during coughs. Little is known about frequency and intensity of influenza infection in the distal airways in mild-moderate influenza illness. Current breath samplers measure shedding, but not whether shedding is driven by intensity of infection or of aerosol generation. Our objective is to determine the concentration of infectious virus in lung lining fluid by collecting exhaled breath. Viral loading is defined as the ratio of the virus amount in the collected aerosol to the volume of the collected aerosols. We recruited 10 individuals with qRT-PCR confirmed ARI to give 10-minute breath samples. We used a novel exhaled breath aerosol (EBA) collector. This system uses condensation growth to collect aerosols ≥ 9 nm and impact them on ice. Participants wore a nose clip, breathed particle-free humidified air and repeatedly exhaled slowly to residual volume then inhaled to total lung capacity. We characterized aerosol number and size distributions with an aerodynamic particle sizer and scanning mobility particle counter and computed volume of the collected aerosols including corrections for humidity changes and sampling losses. Following collection, EBA samples were thawed, transferred to an Eppendorf tube and immediately refrozen and stored at -80°C until analysis. The one participant infected with influenza A H3, exhaled ~ 10 particles/cm³ (GM= 158 nm, GSD= 1.5). The total exhaled aerosol volume over a 10 minute sample was 41×10^{-12} liter. We detected 1.67×10^4 RNA copies. Lung viral loading was 4.12×10^{11} copies/ml. Results from participants with other viral infections are pending.

11CA.1

Experimental Evidence of the Lensing Effect Suppression for Atmospheric Black Carbon Containing Brown Coatings. VAIOS MOSCHOS, Robin Modini, Joel Corbin, Dario Massabò, Silvia G. Danelli, Camilla Costa, Athanasia Vlachou, Kaspar Daellenbach, Paolo Prati, Martin Gysel, Andre S.H. Prévôt, Urs Baltensperger, Imad El Haddad, *Paul Scherrer Institute*

Accounting for the wavelength- and source-dependent optical absorption properties of the abundant light-absorbing organic (brown) carbon (BrC) and the mixing state of atmospheric black carbon (BC) are essential to reduce the large uncertainty in aerosol radiative forcing. Estimation of BrC absorbance online by subtraction is highly uncertain and may be biased if not decoupled from the potential BC absorption enhancement (lensing) due to non-refractory (organic and inorganic) coating acquisition.

Here, the reported total particulate absorbance is based on long-term, filter-based seven-wavelength Aethalometer (AE33) data, corrected for multiple scattering effects with Multi-Wavelength Absorbance Analyzer (5λ MWAA) measurements. Using ultraviolet-visible spectroscopy absorbance measurements along with particle size distributions obtained by a scanning mobility particle sizer, we have conducted optical closure calculations to assess the importance of source-specific extractable particulate BrC¹ versus BC absorbance. The wavelength dependence of bare BC absorption is estimated using MWAA measurements upon successive filter extractions to remove the influence of BrC/coatings. The lensing contribution, supported by observations from field-emission scanning electron microscopy, is estimated at longer wavelengths using a proxy for the BC coating thickness.

Based on the observational constraints and independent modeling approaches, we demonstrate that the interplay between lensing and BrC absorption results in lower than expected BC absorption at shorter wavelengths. This indicates that the volume additivity assumption is not valid for particulate absorption by internally-mixed heterogeneous atmospheric aerosol populations. These comprehensive experimental analyses verify the lensing suppression predicted for core-shell structures containing moderately absorbing BrC². The implications discussed in this presentation are relevant for co-emitted species from biomass burning or aged plumes with high BrC to BC mass/absorbance ratio.

[1] Moschos V, *et al.* (2018) *ES&T Lett.* **5**, 302.

[2] Lack DA, Cappa CD. (2010) *ACP.* **10**, 4207.

11CA.2

Evolution of the Light-absorption Properties of Brown Polycyclic Aromatic Hydrocarbons Due to Reaction with Nitrate Radicals. ZEZHEN CHENG, Khairallah Atwi, Anita Avery, Manjula Canagaratna, Philip Croteau, Edward Fortner, Jordan Krechmer, Francesca Majluf, Leah Williams, Zhenhong Yu, Douglas Worsnop, Andrew Lambe, Rawad Saleh, *University of Georgia*

We have previously shown that brown carbon (BrC) in combustion emissions exhibits a continuum of light-absorption properties that depend on combustion conditions and that polycyclic aromatic hydrocarbons (PAHs) constitute an important fraction of this BrC. Here, we investigate the evolution of these brown PAHs following oxidation by nitrate radicals (NO₃).

We conducted toluene combustion experiments controlled at different conditions to produce PAHs with variable light-absorption properties. We exposed the PAHs to NO₃ in an oxidation flow reactor, where the NO₃ exposure varied from 0 to ~5×10¹³ molec cm⁻³ sec, equivalent to approximately 24 hours of atmospheric exposure. We performed measurements of the chemical composition, size distributions, and absorption coefficients of the fresh and aged aerosols and retrieved the imaginary part of the refractive indices (k) from the light-absorption and size distribution measurements.

Starting with light PAHs (k at 550 nm, k₅₅₀ = 0.007), exposure to NO₃ led to significant darkening (50% increase in k₅₅₀) of the oxidation products at maximum exposure. However, exposure of dark PAHs (k₅₅₀ = 0.08) to NO₃ led to negligible change in light-absorption properties. This discrepancy may be attributed to two competing effects: 1) formation of oxidation products that lead to an increase in k₅₅₀ (e.g., nitro-PAHs), and 2) formation of oxidation products that are less absorbing than the original compounds and therefore reduce the effective k₅₅₀ of the oxidized aerosol as has been observed with OH oxidation. It appears that effect (1) is more prominent for the light PAHs, while the two effects have similar importance for the dark PAHs.

These results indicate that NO₃-induced oxidation darkens some types of atmospheric BrC, which can counterbalance bleaching effects induced by OH oxidation. Furthermore, the light-absorption properties of different BrC components evolve differently in the atmosphere.

11CA.3**Evaluation of the Density and Absorption Properties of Laboratory-Generated Particulate Organic Nitrates (pON).**

JEAN-EUDES PETIT, Alexandre Albinet, Andrew Lambe, Athina-Cerise Kalogridis, Liine Heikkinen, Frans Graeffe, Manuela Cirtog, Anaïs Féron, James Allan, Zainab Bibi, Tanguy Amodeo, Nicolas Karoski, Robin Aujay-Plouzeau, Laurent Meunier, Valerie Gros, Nicolas Bonnaire, Roland Sarda-Esteve, Francois Truong, Mikael Ehn, Tuija Jokinen, Minna Aurela, Evelyn Freney, Leah Williams, Olivier Favez, et al., *LSCE*

Atmospheric particulate organic nitrates (pON) have recently been shown to account for a large fraction of organic aerosol (OA). Through light absorption, especially at short wavelengths, they make up part of atmospheric brown carbon. While pON might be a non-negligible climate-forcing agent, the physical and optical properties are still poorly documented. As part of the Aerosol Chemical Monitor Calibration Centre (ACMCC) pON experiment, measurements have been conducted to characterize the physical and optical properties of laboratory-generated pON, such as density, mass absorption coefficient (MAC) and refractive index (RI). pON were generated in a Potential Aerosol Mass oxidation flow reactor from the reaction of single VOC precursors with NO₃ radical, using two biogenic (limonene and β -pinene) and two anthropogenic (acenaphthylene and guaiacol) compounds. In addition to online physicochemical characterization with aerosol mass spectrometers, a suite of instruments was dedicated to study the physical and optical pON properties, including an aerodynamic aerosol classifier (AAC), a centrifugal particle mass analyzer (CPMA), a scanning mobility particle sizer (SMPS), a condensation particle counter (CPC) and a multi-wavelength aethalometer (AE33). Results will be discussed according to different precursors (biogenic/anthropogenic), as well as compared to the literature data from laboratory experiments for the same (and other) precursors but in different chemical conditions, such as OH or NH₃ exposure. Results for laboratory-generated pON will also be compared with ambient air observations.

11CA.4**Quantifying Organic Matter and Functional Groups in Aerosol Filter Samples from the Southeastern Aerosol Research and Characterization (SEARCH) Network.**

ALEXANDRA BORIS, Satoshi Takahama, Andrew Weakley, Bruno Debus, Stephanie L. Shaw, Eric Edgerton, Ann Dillner, *University of California, Davis*

A broad view of atmospheric aerosol organic matter (OM) composition is afforded by Fourier transform infrared (FT-IR) spectrometry of filter-based samples. Infrared absorption patterns and multivariate calibration efficiently quantifies OM and functional group quantities on individual samples. Teflon filter samples are analyzed quickly and without damage, enabling application to air monitoring networks as well research campaigns. This methodology is an improvement over OM calculated by converting routinely measured organic carbon (OC) concentrations to OM using a constant OM/OC ratio.

This work discusses the contribution of functional groups to OM, as well as total OM concentration, directly measured within samples from the Southeastern Aerosol Research and Characterization (SEARCH) network. The study expands upon previous work to include particle water, additional oxygenated chemical standards, and improved functional group specificity (e.g., addition of carboxylates). The ~5400 SEARCH samples collected over eight years (2009-2016) allow contrast between urban and rural compositions, between months, and over a long time period. Preliminary results demonstrate that FT-IR spectrometry measured composition matches that from other techniques, including in the van Krevelen space and relative to residual OM (calculated using aerosol mass balance from network measurements). Long-term trends are observed in OM concentration and composition, as are seasonal differences in OM degree of oxidation. This work is a step toward quantifying all major functional groups and evaluating variability of total OM composition.

11CA.5**Regional Climate and Air Quality Impacts of Particulate Emissions from Gasoline Direct-Injection (GDI) Vehicles.**

SOROUSH ESMAEILI NEYESTANI, Gabriel Kooperman, Rawad Saleh, *University of Georgia*

Due to their enhanced fuel economy, the market share of Gasoline Direct-Injection (GDI) 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. The competing effect of reducing carbon dioxide emissions but increasing BC emissions raises a question regarding the net climate impacts of GDI vehicles. 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 used the Weather Research and Forecasting model coupled with chemistry (WRF-Chem), which simulates both chemical transport and radiative transfer. The simulations were performed at a 12 km resolution and for a period of two months (January and July) in 2011 to take into account the seasonal variability. Using the EPA's National Emission Inventory (NEI) for 2011 as a base case, we modified the vehicle emission profiles using GDI emissions data obtained from measurements. By comparing the base case (PFI) with the modified one (GDI), we calculated changes in carbonaceous aerosol concentrations and the consequent radiative effect. Our results indicate that shifting the fleet to GDI vehicles leads to a net warming effect over the U.S., with radiative effect as large as 0.5 W/m^2 over cities with high transportation activity. Furthermore, using $\text{PM}_{2.5}$ concentrations obtained from the simulations and the concentration-response factor employed by EPA, we calculated spatially resolved $\text{PM}_{2.5}$ caused mortality rates. The results indicate that due to the increase in $\text{PM}_{2.5}$ emissions, a shift from PFI to GDI would double the rate of premature deaths attributed to gasoline vehicle emissions.

11CA.6**Seasonal Variations in Aerosol Emissions from Light- and Heavy-Duty Vehicles in the Fort McHenry Tunnel.**

ANDREY KHLYSTOV, David Campbell, *Desert Research Institute*

Vehicular traffic is one of the main sources of particulate matter and its precursors. Due to the introduction of increasingly stringent emission standards, significant advances in automotive technology and fuel formulations were made in recent years. We will present results of a study aimed to investigate real life effectiveness of emission controls and to update profiles of traffic-emitted air pollutants. The study was conducted in the Fort McHenry Tunnel in Baltimore, MD, during two one-week-long campaigns, one in winter (February 2015) and one in summer (August 2015). The tunnel passes under the Baltimore Harbor, carrying traffic of Interstate 95, approximately 55,000 vehicles per day. UFP size distributions were measured using scanning mobility particle sizers, while aerosol chemical composition was measured using filter-XAD pairs to capture both particle- and gas-phase semivolatile compounds. Filter and XAD samples were analyzed using gas chromatography – mass spectrometry for polycyclic aromatic hydrocarbons (PAH), alkanes, hopanes, steranes, and nitro-PAHs. Carbon monoxide, nitrogen oxides, and volatile organic compounds were also measured. Emission factors (EFs) of over 400 pollutants were determined separately for light duty (LD) and heavy duty (HD) vehicles during winter and summer seasons of 2015. Warm and cold season measurements allowed us to assess the effect of temperature on UFP size distributions and EFs of different pollutants. The EFs measured during this study will be compared with those from earlier real-world emission measurements in the U.S.A. in which EFs for LD and HD vehicles were reported separately, including a 1992 study conducted at the Fort McHenry Tunnel. The present study provides a check on whether emissions in the East Coast of the U.S.A. experienced similar emission reductions as California, where most past traffic emission studies took place. A comparison with predictions by the MOVES2014 model will also be presented.

11CO.1

It's Not All about Mass: Changes in Particle Number and Composition from Light Duty Vehicle Engine Combustion through the Use of Gasoline Particle Filters. REBECCA TANZER GRUENER, Stani Bohac, Albert A. Presto, *Carnegie Mellon University*

Gasoline particle filter (GPF) technology has been implemented in all 2019 light duty vehicles (LDVs) in Europe that use direct injection as the sole method of fueling. GPFs will also be appearing on LDVs in China within the next year. GPFs reduce particulate matter (PM) mass, number, nanoparticles, black carbon, and exhaust toxicity. However, GPFs are not expected on U.S. vehicles in the near term because the U.S. does not currently regulate particulate number. To inform the development of future emissions regulations in the U.S. a test program is being conducted to assess the effects of utilizing this technology. PM emissions from a 2011 F150 truck with a 3.5L Ecoboost GDI engine are being analyzed during start-up, idling, and various drive cycles, with and without an underfloor GPF retrofit to the vehicle. Experiments are being run on a chassis dynamometer using Tier 3 fuel at various laboratory temperatures (20, 50, and 70 degrees F). Particle mass is analyzed using Teflon filters, carbonaceous material is measured using micro soot samplers (MSS), and particle number and size distribution is quantified using an engine exhaust particle sampler (EEPS). PM samples collected on quartz filters are being used for carbon analysis using an OCEC analyzer and additional quartz filters are used for GC-MS analysis of volatility of the exhaust. Gas-phase and particle-phase exhaust SVOC speciation is conducted to quantify the GPF's effect on polycyclic aromatic hydrocarbon (PAH) emissions and toxicity, as well as to better the understanding of the effect of GPFs on SOA precursors. Quantifying the difference in exhaust composition with and without the use of the GPF will lead to a greater understanding of this combustion emissions mitigation technology.

11CO.2

Exploring the Secondary Organic Aerosol Formation Potential and Subsequent Secondary Trends from Gasoline Direct Injection Vehicles with Varying Experimental Conditions. PATRICK ROTH, David R. Cocker III, Georgios Karavalakis, Akua Asa-Awuku, *TSI Incorporated*

The goal of this work was to aggregate the data collected from all vehicle exhaust irradiation experiments utilizing UCR's Mobile Atmospheric Chamber (MACH), and attempt to explain trends in the secondary aerosol formation. This aggregation contains data from four independent studies measuring the secondary organic aerosol (SOA) formation from new technology, low mileage, gasoline direct injection (GDI) vehicles. The data set includes nine vehicles, in 36 testing configurations, and 88 individual tests. These studies explored the emissions from stock vehicle configurations, additional after-treatment configurations, and vehicles operating on varying fuel compositions.

No trends with the formation of inorganic salt were found with either NO_x or NH₃ indicating both reactants can act as the limiting reagent in the salt formation. The SOA formation potential measured in this work were right in line with previous experiments with chambers exploring the secondary potential of vehicle exhaust. We observed a decrease in the SOA potential of the vehicle exhaust as the certification standard increased. Similarly as the ethanol content of the fuel increased, so did the secondary organic aerosol potential.

In regards to observed trends in the exhaust, as NMHC emission factors increased, so did the SOA formation potential. The trend was very strong in emissions over 20 mg/mi however there was much more variability in the lower emission levels.

The yield of the vehicle exhaust was also explored, and the trend was quite broad when looking at all tests as a whole. However, when exploring the similar reaction conditions, it was found that when tests were split by VOC:NO_x emission ratios, the corresponding yield changed based on the ratio. More relationships with the yield and various concentrations were also explored.

11CO.3**Characterizing In-Use Commercial Harbor Craft Emissions.**

CHELSEA V. PREBLE, Rebecca Sugrue, Hannah Schlaerth, George Ban-Weiss, Thomas W. Kirchstetter, *University of California, Berkeley*

As on-road diesel fleets increasingly adopt diesel particle filters (DPFs) and selective catalytic reduction (SCR) emission control systems, off-road sources like marine vessels will become increasingly important contributors to total diesel PM and NO_x emissions. Diesel-related pollution from commercial harbor craft—including ferries, tugboats, and fishing vessels—can negatively impact the air quality and health of near-shore communities. Current emission inventories and regulatory planning efforts assume engine certification emission rates for these commercial harbor craft. However, previous work with the on-road diesel truck fleet shows that a minority of in-use vehicles can emit at levels well above certification limits and dominate total fleet emissions. As such, there is a need to characterize the in-use emissions from these vessels so as to better inform PM, NO_x, and greenhouse gas emissions reduction efforts in this sector.

Emissions from in-use commercial harbor craft operating in the San Francisco Bay are measured using the plume capture, carbon balance method. Measurements are made on-board multiple vessels in coordination with their operators. Sampled vessels include engines with and without DPF and SCR systems that meet EPA Tiers 2–4 emission standards. These measurements capture a variety of operating conditions, including steady cruise emissions and variable berthing emissions. Preliminary fuel-based black carbon (BC) and NO_x emission factors (g emitted per kg of diesel consumed) are lower and higher, respectively, for diesel powered ferries than heavy-duty diesel trucks with comparable control technologies. Emission factors are related to vessel speed and acceleration via concurrently tracked GPS data; the carbon footprints of commuting by ferry versus by car are also compared.

11CO.4**Impacts of Switching from Diesel to Liquefied Natural Gas (LNG) for A Marine Vessel.**

WEIHAN PENG, Jiacheng Yang, Joel Corbin, Qi Li, Una Trivanovic, Steven Rogak, Prem Lobo, Patrick Kirchen, Stephanie Gagne, David R. Cocker III, Wayne Miller, *University of California, Riverside*

Ship owners are challenged to meet ever more stringent standards for criteria pollutants and greenhouse gases (GHG). To meet those goals, the manufacturers of trucks, buses and cars have shown that operating on natural gas reduced both criteria pollutants and greenhouse gases; however, little is known about switching from diesel to natural gas in marine vessels. In this project, the emissions from a modern large ferry's dual-fuel engine operating on natural gas in the Tier 3 mode and operating on diesel in the Tier 2 mode were compared.

We measured particle size distributions and black carbon (BC) emissions, and found that the emitted particles were associated with the lubrication oil (the majority of mass) or the diesel pilot fuel (majority of BC) for both fuels. We also measured emissions of criteria pollutants (PM_{2.5}, CO, SO_x, NO_x), EC/OC, carbonyls, CH₄, and CO₂ from the vessel for various engine loads. Switching from diesel to LNG reduced PM_{2.5} mass by 93%, BC by 97%, CO₂ by 18%, and NO_x by 93%, however, emissions increased for incomplete combustion products (CO and HCHO) and unburned CH₄. A health risk assessment showed that diesel was more harmful when considering carcinogenic and chronic health effects from both PM and HCHO. An analysis of the GHG and BC emissions was performed and found that, on 100-year basis, LNG's GWP per kWh was higher than diesel's at lower loads, but that it was similar at 75% engine load and better at higher loads. Since CH₄ emissions may be reduced by technological advances, LNG has the potential to be a lower-GWP fuel than diesel in the future, in addition to its health benefits. Mitigation strategies for further reducing pollutants from LNG exhaust were discussed, with emphasis on reducing the increased pollutants i.e. CO, HCHO and CH₄.

11CO.5

Uncertainty in Thermal-Optical Analysis for Elemental Carbon from Aircraft Engine Exhaust. GREGORY SMALLWOOD, Stephanie Gagne, Brett Smith, Joel Corbin, Benjamin Brem, Andrea Fischer, Lukas Durdina, Prem Lobo, *National Research Council Canada*

The real-time instruments used for regulatory measurements of aircraft engine non-volatile Particulate Matter (nvPM) mass emissions have to be calibrated to the mass of elemental carbon (EC) determined by thermal-optical analysis (TOA) of the filter-sampled emissions of a diffusion flame source. This EC is defined by an analysis method originally based on the National Institute of Occupational Safety and Health (NIOSH) Method 5040 for diesel PM. This method involves evaporating volatile organic carbon in an inert helium environment and non-volatile carbon in a helium-oxygen environment, while monitoring the filter transmittance to evaluate a pyrolysis correction to determine a so-called split point between organics and EC. However, significant differences have been observed in the EC content determined by different laboratories. These differences are observed as bias between different laboratory analyzers, differences in split-point assignment, and greater scatter on some laboratory instruments compared to others. To investigate the differences observed in the TOA results and determine the associated uncertainties, we performed a set of round-robin experiments following the standard procedures for determining EC mass concentration as described in SAE ARP6320. A total of 20 filter samples were acquired from the exhaust of a Rolls-Royce Gnome engine. Six punches from each filter were distributed amongst the five laboratories (one laboratory performed duplicate analyses), each following the standard TOA protocol defined in SAE ARP6320. Preliminary results indicate that the variability between different laboratories for EC was $\pm 11.4\%$ with a standard deviation of $\pm 2.6\%$. A separate two-way comparison was also performed on filter samples collected for nvPM emissions from a CFM56-7B engine. These results will be used to assess the reproducibility of this method.

11CO.6

Particle Emissions from In-use Commercial Aircrafts Observed at the Narita International Airport. NOBUYUKI TAKEGAWA, Kentaro Misawa, Akihiro Fushimi, Yoshiko Murashima, Hiromu Sakurai, *Tokyo Metropolitan University*

Jet-engine aircrafts are important sources of ultrafine aerosol particles in the atmosphere. Intensive measurements of aerosols and combustion tracer gases (carbon dioxide (CO₂) and nitrogen oxides) were conducted at an observation point ~140 m from the major runway of the Narita international airport, Japan between February 7 and 23, 2018. The number concentrations of aerosol particles with diameters larger than 2.5 nm (N_{2.5}, TSI-UCPC3776), those larger than 10 nm (N₁₀, TSI-CPC3771), and mixing ratio of CO₂ are used to estimate the effective particle number emission factors from in-use commercial aircrafts under real-world operating conditions. The inlet tube for the UCPC and CPC was switched between unheated (room temperature) and heated (350 degrees C) modes every 8 h. The sampling method for heated N₁₀ corresponds to the standard procedure for aircraft engine exhaust measurements (SAE AIR6241). The consistency between our measurements and the standard procedure was tested in the laboratory before and after the intensive observation period. Except for specific time slots with frequent aircraft traffics at the runway, we successfully identified isolated plumes from individual aircrafts based on spiked increases in CO₂ (>100 plumes both for unheated and heated modes). A comparison between unheated or heated N_{2.5} and N₁₀ in those plumes indicates that the particle number emissions were dominated by volatile particles with diameters smaller than 10 nm. For some selected cases, the observed plumes were further classified into take-off and landing events based on detailed flight information provided by the airport. The sampling distances of the observed plumes were estimated using local wind data. Variability in the effective number emission factors is discussed in relation with the estimated sampling distances, landing/take-off cycles, and aircraft types. Similarities and differences between our results and earlier studies are also discussed.

11IS.1

Secondary Aerosol Mass Contributions from Human Occupants in a Classroom. ANITA AVERY, Michael Waring, Peter DeCarlo, *Drexel University*

Humans can impact the composition of indoor air via heterogeneous reactions of gas-phase oxidants with skin constituents on an occupant or skin that has been shed (desquamation), as well as by direct emissions from people themselves (bioeffluents) and the personal care products they use. However, separating the influence of the many emissions and their oxidation products from the influence of outdoor-originated aerosols has been a challenge. Indoor and outdoor aerosols were alternatively sampled at 4-minute time resolution with a high-resolution time-of-flight aerosol mass spectrometer (HR-ToF-AMS) in a classroom with student occupants at regular intervals. Mass spectral analysis showed aerosol enhancements of oxidized and unoxidized hydrocarbon ion families during occupied periods, especially at ion fragments larger than m/z 100 and double bond equivalents consistent with squalene ($C_{30}H_{50}$) and its oxidized products from reaction with ozone, indicative of the secondary nature of the aerosol mass. Individual hydrocarbon mass fragments consistent with squalene fragmentation, including $C_5H_9^+$, and $C_6H_9^+$ were especially enhanced with room occupancy. Other oxidized fragments related to oxidation products of squalene and ozone were also enhanced. Emissions of individual organic fragment ions were estimated using a model accounting for outdoor aerosols and air exchange. This showed occupancy related emissions at smaller fragments from occupants indoors. Ozone losses (β) were used to parameterize emissions to relate to other environments, such that total emission of all fragments was $17.6 \mu\text{g } \beta^{-1} \text{ h}^{-1}$ above unoccupied levels. This translates to approximately 25% increase in organic aerosol mass concentration in the classroom during an occupied hour with a median occupied ozone loss. Human occupants, therefore, represent an additional mass burden of organic aerosol, especially in poorly ventilated or highly occupied indoor spaces.

11IS.2

Post-Wildfire Assessment of Indoor Dust Composition in Canadian Homes. JUSTIN H. DINGLE, Lukas Kohl, Meng Meng, Yue Shi, Arthur W. H. Chan, *University of Toronto*

Indoor house dust is a source of human exposure to persistent pollutants and is linked to potential health risks. The Fort McMurray, Alberta wildfire event in May 2016 raised questions about potential exposure to fire-related pollutants. To assess the long-term impacts of the wildfire emissions and any other sources on indoor air quality, dust was collected in Fort McMurray homes during four sampling campaigns in 2017-2018 and the concentrations of trace elements were analyzed. Dust samples were acid digested and characterized for 25 trace metal elements using Inductively Coupled Plasma Mass Spectrometry. The dust collected in the bedroom, basement, and entryway highlight characteristics that shows distinct trace metal element dominating in specific locations of the house. Cu, Zn, and Pb sampled in basement areas were increased on average by a factor of 2-3. However, Na, Mg, Al, K, and V were increased by \sim 56-90, 5-110, 20-125, 30-40, and 70-160 % in the entryway compared to other location of the homes, respectively. Bedroom samples showed the lowest concentrations for 22 out of 25 metals characterized in the dust samples except for Cd, Sb, and Ag being 35, 50 and 110% increased compared to samples collected in the entryway, respectively. Concentration levels were compared to the Alberta Tier 1 regulatory limits and generally fell within the guidelines. Enrichment factor ratios (EF) for indoor trace metal elements were calculated to compare concentrations of indoor dust samples with soil concentrations found in areas near oil sands operations and soils isolated from human activities (baseline soils) in the Fort McMurray area. Considering EF close to 1 representing metals similar to outdoor soils, EF for Cu, Zn, Cd, and Sb in entryway dust were \sim 8, 7, 6, and 10 respectively while in basement dust the EF for Pb was 6.

11IS.3

The CHEER Study: It's a Complicated Association between Home Infiltration Rates and Respiratory Health. SHELLY MILLER, Jamie Humphrey, Prateek Shrestha, John Adgate, Elizabeth Carlton, Elisabeth Root, *University of Colorado Boulder*

In the Colorado Home Energy Efficiency and Respiratory Health (CHEER) study we evaluated the relationship between home air-tightness, infiltration rates and characteristics, and occupant respiratory health of low-income homes across the Front Range of Colorado. Respiratory questionnaires, lung function testing, household walkthrough inspection, and blower door testing were used. An additional study was conducted over two summers investigating the impact of wildfires on indoor air quality in our study homes.

In summary, we found that in the questionnaire study homes with lower annual average infiltration rates (AIR) reported fewer respiratory symptoms. Furthermore, we suggest based on our analyses that one reason we see this association is because traffic-related air pollution is infiltrating the homes and impacting respiratory health as reported by questionnaire. Most of our homes were fairly leaky and had their windows open quite a bit especially during nice weather.

Conversely in the spirometry study we found that high AIR may be beneficial for lung health. These results are more in line with previous studies. Note that the CHEER study by design sampled from low income, urban populations who are disproportionately burdened by respiratory illness. The study population in this study was more limited since many of the "sickest" could not perform the spirometry test. Thus, the spirometry sample is a healthier population compared to the questionnaire sample and perhaps less susceptible to subtle changes in air quality.

Investigations into the impacts of energy efficiency retrofits designed to tighten the building structure revealed that although these efforts did have an impact on lowering the AIR, the most significant factor determining air exchange was building volume and age. Duct sealing turned out to be quite effective as a retrofit.

The wildfire study showed that indoor levels of PM_{2.5}, CO and black carbon were significantly impacted by the smoke plume. Of note was the fact that almost all homes kept their windows open and did not have air conditioning.

In an additional analysis to understand neighborhood characteristics as a whole we found four distinct types of neighborhoods and that these typologies can impact respiratory health.

Outcomes of this study will provide guidance on air-tightness and energy efficiency upgrade techniques that reduces energy use in homes while still providing a healthy indoor environment.

11IS.4

Outside-In and Other Sources of Aerosols in the Indoor Environment. PETER DECARLO, Anita Avery, Erin Katz, Michael Waring, Marina Vance, Delphine K. Farmer, *Drexel University*

Combining high time resolution indoor and outdoor measurements of particle composition by aerosol mass spectrometry from both studies performed in a university classroom, and the "HOMEChem" (House Observations of Microbial and Environmental Chemistry) project, we investigate the various sources and processes which contribute to indoor aerosols. For both the classroom and HOMEChem project, indoor particle mass concentrations are typically lower than outdoor concentrations in the absence of large indoor sources (e.g. cooking activities). Compositional changes for outdoor-to-indoor transported aerosol is observed and can be linked to changes in relative humidity (RH) and temperature (T) gradients between the outdoor and indoor environments (e.g. particle nitrate volatilization) when indoor T exceeds outdoor T. Additionally, unique indoor sources can be identified from residual cigarette smoke, human occupants, cooking, and cleaning activities. Residual cigarette smoke contribution to indoor aerosol was identified in a non-smoking building and contributed up to 30% of the indoor aerosol mass during warmer months when air conditioning (AC) was employed. During months when the building air supply was heated this component was not identified, and this difference is attributed to residual smoke chemical species partitioning to the liquid water phase of indoor aerosols present in summer (with AC), but not in winter. Human occupant contributions to secondary organic aerosol mass was identified during periods of high occupancy (elevated CO₂) and enhanced indoor ozone loss in the classroom studies. Cleaning activities during HOMEChem also showed chemical changes to indoor aerosol composition, although mass enhancement was small. Finally cooking activities during HOMEChem showed the largest increases in indoor particle mass loadings and greatly exceeded outdoor levels. A significant fraction of this mass was chemically similar to cooking oils. The relative contribution of these various sources will be discussed.

11IS.5

Spatial Distribution of Indoor Aerosol during HOMEChem Cooking Events. ERIN K. BOEDICKER, Delphine K. Farmer, Marina Vance, *Colorado State University*

Cooking is a major contributor to fine (100 nm – 2.5 μm) and ultrafine (<100 nm) aerosol concentrations indoors. Understanding the indoor dynamics that impact these aerosols is crucial in order to assess overall human exposure. This work aims to further characterize aerosol emissions from cooking, investigate the spatial and temporal gradients caused by the mechanisms of aerosol transport indoors, and determine the major loss mechanisms for particles indoors. In order to probe these different elements of indoor aerosol sources a variety of cooking experiments (e.g. stir-fry, toast, chili, etc.) were conducted during the House Observations of Microbial and Environmental Chemistry (HOMEChem) campaign. The emissions from these experiments were measured using size resolved optical instruments at four points throughout the house simultaneously. During background periods, aerosol concentration indoors was, on average, $50 \pm 10\%$ lower than the observed outdoor concentration, however, during cooking events the concentration indoors was measured to be $70 \pm 30\%$ to $180 \pm 20\%$ higher than outdoors, depending on the room and the cooking event. The majority of particles emitted during these events were less than 100nm in diameter (CMD ranged from 85 to 170 nm depending on the cooking experiment). After emission, the particles took approximately 0.7 ± 0.1 minutes to reach the living room, with a $60 \pm 10\%$ decrease in concentration, and they took 2.4 ± 0.9 minutes to reach the bedroom, with an $87 \pm 2\%$ reduction in concentration. Deposition was found to be the dominate loss process with loss rates ranging from 0.00005 to 0.0005 s^{-1} and deposition velocities ranging from 0.02 to 0.05 m/s depending on size of the particles.

11IS.6

Insights on Aerosol Emissions during HOMEChem. SAMEER PATEL, Sumit Sankhyan, Yilin Tian, Allen Goldstein, Delphine K. Farmer, Marina Vance, *University of Colorado Boulder*

In the US, people spend about 90% of their time in indoors¹, and indoor $\text{PM}_{2.5}$ exposure has been estimated to account for more than a quarter of fine particulate matter (PM) mortality burden highlighting the importance of focusing more on IAQ in the developed world². Much of indoor PM exposure—in addition to outdoor penetration—is due to indoor activities such as cooking. Aerosol emissions from cooking are relatively less investigated in developed countries compared to developing countries which rely on solid fuels for cooking and space heating.

We conducted an indoor chemistry field study titled HOMEChem (House Observations of Microbial and Environmental Chemistry). IAQ in a three-bedroom, two-bathroom 110 m^2 manufactured test house was comprehensively characterized while everyday activities such as cooking, cleaning, and opening doors and windows were performed. $\text{PM}_{0.1}$ and $\text{PM}_{2.5}$ exceeded $100 \mu\text{g m}^{-3}$ and $300 \mu\text{g m}^{-3}$, respectively, during some cooking events. Estimated mass of PM deposited in the respiratory system of an adult residing in the test house during a experiments simulating a routine day (breakfast, lunch, and dinner followed by cleaning activities) and a typical Thanksgiving meal preparation were almost nine times (62.3 μg) and 17 times higher (129 μg), respectively, compared to a day with no activities (7.4 μg).

The formation and growth of sub-30 nm particles were observed after mopping the floors with bleach but only when a specific type of meal preparation preceded mopping. Such observations indicate particle formation governed by the chemistry between certain species originating from both cooking and cleaning.

[1] Klepeis et al. (2001), *Journal of Exposure Science and Environmental Epidemiology*.

[2] Azimi and Stephens (2018), *Journal of Exposure Science & Environmental Epidemiology*.

12AC.1**Sulfate Formation from SO₂ Uptake onto Organic Aerosol.**

Shunyao Wang, William Tsui, V. Faye McNeill, Jonathan Abbatt, ARTHUR W. H. CHAN, *University of Toronto*

Particulate matter is dominated by sulfate and organic aerosol (OA). Secondary formation of these components are often studied and modeled separately, but the observed correlations between their concentrations suggest synergistic reactions. Previous laboratory studies show that secondary organic aerosol (SOA) yields are higher when formed in the presence of SO₂, but the mechanisms by which SO₂ reacts are not known. In this work, we conducted bulk solution experiments of S(IV) oxidation by organic peroxides to investigate the kinetics and mechanisms of sulfate formation, and chamber experiments of SO₂ uptake onto peroxide-containing OA.

The bulk reaction rate constants of SO₂ with commercially available organic peroxides (cumene hydroperoxide, benzoyl peroxide and 2-butanone hydroperoxide) are quantified as a function of pH, and are shown to be similar to that with H₂O₂. Using isotopically labeled reagents and ion-mobility mass spectrometry (IMS-TOF), we show that organosulfates are formed from ROOH + SO₂ at a substantial yield of 40%. This mechanism is unique from previously proposed pathways for organosulfate formation, which require inorganic sulfate as a reactant. Further experiments are conducted in the aerosol phase by generating SOA in the flow tube and measuring SO₂ uptake onto SOA in the chamber. The uptake coefficients are measured for different SOA containing different types and amounts of organic peroxides. Organosulfate speciation using IMS-TOF is examined and compared to the backbone of SOA precursors. The mechanisms and kinetic parameters derived from this work are applied in an aerosol kinetic model (GAMMA) to understand the rate of SO₂ uptake and inorganic and organic sulfate formation in the aerosol. Preliminary modeling results suggest that this reaction can account for all of the observed SO₂ uptake onto SOA from limonene ozonolysis, and results for other SOA systems and implications on atmospheric chemistry will be discussed.

12AC.2**Moving Beyond the Bulk Phase: Kinetics of SO₂ Oxidation in Sub-Micron, Deliquesced Aerosol Particles.**

TENGYU LIU, Jonathan Abbatt, *University of Toronto, Canada*

Sulfate aerosol is a major component of fine particulate matter and has important impacts on air quality, climate, and human and ecosystem health. However, current atmospheric models that include gas- and aqueous-phase oxidation pathways of SO₂ generally underestimate the sulfate production rate during severe haze events. The reaction rate coefficients for aqueous-phase oxidation pathways in these models have been determined in bulk solution, which may not be applicable to the wet aerosol particles with three to five orders of magnitude lower water content and very much higher ionic strength than that of fog or cloud droplets. Here, we utilize a flow tube system that allows us to directly investigate, to our knowledge for the first time, the aqueous phase oxidation of dissolved SO₂ by H₂O₂ in sub-micron, deliquesced aerosol particles at two different aerosol pH values (2.8 and 5.7) at RH of 74–90% and high ionic strength. The aerosol pH is buffered to minimize the pH changes induced by the sulfate formation. The pH-, SO₂-, and H₂O₂-dependent sulfate formation rates are determined. The kinetics display first-order reactions in sulfur (IV) and H₂O₂, similar to those in bulk solution. Overall, the sulfate formation rates are 2.2 times of the modeled sulfate formation rates from bulk phase studies at both pH values. The flow tube system is also being used to investigate the SO₂ oxidation catalyzed by transition metal ions to give insights on the relative roles of different oxidation pathways during severe haze events. Results from initial studies with transition metal ions will also be presented. Updating the current models with kinetic data for sulfate formation in sub-micron aerosol particles will improve air quality and climate simulations.

12AC.3

Mechanisms and Compounds in Atmospheric Acid-Base Particle Formation. NANNA MYLLYS, Tinja Olenius, Sabrina Chee, James Smith, *University of California, Irvine*

In atmospheric sulfuric acid-driven particle formation, ammonia and amines are the most commonly studied stabilizing compounds. As a stronger base, dimethylamine enhances particle formation rate several orders of magnitude more than ammonia. The base strength seems to be an important factor in particle formation, which leads to the following question: *“Does our atmosphere contain stronger bases which would be more effective in particle formation than amines?”*. Guanidine is a very strong organobase and its cationic form is an extraordinary stable. Guanidine and sulfuric acid form clusters, which have a high symmetry and a large number of intermolecular bonds. Thus, those clusters are very stable against evaporation and particle formation is fully collision driven. Guanidine enhances sulfuric acid-driven particle formation up to eight orders of magnitude more than dimethylamine. Guanidine was used as a model compound, and later found from Hyytiälä boreal forest. This indicates that atmosphere might contain a plethora of other strong bases which can significantly enhance particle formation.

Experimental studies have shown that when combining amines and ammonia together with sulfuric acid, particle formation rates are 10–100 times higher compared to two-component sulfuric acid–amine mixtures. This cannot be explained by base strength, and therefore, we have studied the cluster structures and energetics in order to answer the question: *“What is the fundamental reason for the synergy between ammonia and amines?”*. Even dimethylamine is a stronger base, ammonia is more likely to be protonated in mixed clusters. Ammonium is T_d symmetric and capable of forming four intermolecular bonds. Thus, it can act as a bridge-former in sulfuric acid–dimethylamine clusters. At atmospheric conditions, ammonia-amine synergy might lead up to five orders of magnitude increase in particle formation rates compared to solely amine-enhanced particle formation.

12AC.4

Oxidation of Reduced Sulfurs and Amines: Characterization and Mechanism Development. PAUL VAN ROOY, Kathleen Purvis-Roberts, Philip Silva, Matthew Nee, David R. Cocker III, *University of California, Riverside*

Gas-phase amines (trimethylamine, diethylamine, butylamine, ammonia) and reduced sulfur compounds (dimethylsulfide, dimethyldisulfide) are both present over agricultural land and are both thought to be important to new particle formation and particle growth. Despite this, there is a lack of knowledge on how these compounds oxidize in the atmosphere individually nor is there a mechanism by which these compounds interact to form aerosol. To begin to fill this information gap, a 37.5 cubic meter Teflon chamber was utilized to run hydroxyl radical and nitrate radical oxidation experiments of each compound individually as well as interaction experiments containing at least one amine (100ppb) and one reduced sulfur (100ppb). Methanesulfonic acid is considered an important product of reduced sulfur oxidation however, under extreme dry conditions and in the presence or absence of NO_x , methanesulfonic acid did not form. Measurements made using the HR-TOF-AMS present sulfur-containing organic fragments, such as $\text{C}_2\text{H}_6\text{S}$ and $\text{C}_2\text{H}_6\text{SO}$, that cannot be explained by the current mechanism. Only when humidity as well as NO_x was introduced into the chamber did methanesulfonic acid form. Interestingly, precursor decay was much faster in the presence of NO_x , indicating that $\text{O}(^3\text{P})$ plays an important role in oxidation of reduced sulfurs during chamber experiments, which are often run at high NO_x concentrations. Addition of an amine to the system allows for methanesulfonic acid formation under dry, NO_x -free conditions. Interactions between amines and reduced sulfur compounds results in aerosol mass concentrations up to 10 times higher than individual precursor oxidation. The addition of humidity to interaction experiments resulted in up to 4 times the mass formed during dry experiments. An updated mechanism for reduced sulfur oxidation is proposed along with a particle-forming mechanism for amines in the presence of reduced sulfurs.

12AC.5

Missing Source of Atmospheric Sulfate Formation in Wintertime Beijing Haze: Linking SO₂ Oxidation and HONO Chemistry. JUNFENG WANG, Jingyi Li, Jian Zhao, Jianhui Ye, Xinlei Ge, Yiming Qin, Pengfei Liu, Shaojie Song, Hong Liao, Mindong Chen, Yele Sun, Qi Zhang, Scot T. Martin, Daniel Jacob, *Harvard University*

Sulfate comprises a large fraction of atmospheric fine particulate matter and exerts nontrivial impacts on regional air quality and global climate. Current atmospheric models with known mechanisms often fail to explain the high sulfate levels observed under complex environmental conditions. An intensive field campaign was conducted during the winter time of 2016 (December 16 to December 23) in Beijing, and formation of secondary sulfate was investigated.

Compared to the less-polluted days, secondary sulfate concentration increased by nearly two times during a severe fog-haze event. We found that sulfate concentrations correlated tightly with HONO as well as N₂O concentrations in fog-haze days, suggesting a sulfate formation pathway: $2\text{HONO} + 2\text{H}_2\text{SO}_3 \rightarrow 2\text{H}_2\text{SO}_4 + \text{N}_2\text{O} + \text{H}_2\text{O}$. The reaction takes place in aqueous particles with HONO acting as an oxidant to transform S(IV) to S(VI) and N₂O formed as a tracer product.

This novel sulfate formation pathway in the presence of HONO was further examined by using a chemical box model and a regional-scale model (i.e., Community Multiscale Air Quality Modeling). Results demonstrate that the enhancement of sulfate formation in the droplets (liquid water contents of 0.1-0.5 g m⁻³) under foggy conditions was closely associated with HONO, and matched well with the observed sulfate concentrations. The work presented herein highlights a long-ignored secondary source of atmospheric sulfate and a potential sink of nighttime atmospheric HONO.

12AP.1

Monte Carlo Simulations of Particle Formation Processes. GREGOR KOTALCZYK, Ivan Skenderović, Frank Einar Kruijs, *University Duisburg-Essen*

We discuss the application of Monte Carlo (MC) simulation techniques for the description of typical particle production processes. The discussed modelling techniques encompass the decomposition of a precursor, which leads to the formation of a metallic vapour. Different temperature profiles (especially cooling rates) lead to a drastic increase of a supersaturation and thus to the onset of the nucleation of novel particles as well as their subsequent growth due to condensation and coagulation. The evaporation of particles has also to be taken into account in certain simulation scenarios, especially in those, in which temperature profiles (originating from turbulent carrier gas flows) describe an increase of the temperature after the nucleation took place and thus to the formation of unstable particles (i.e. whose diameter is smaller than the Kelvin diameter).

In a first part, we give a quick overview of the applied simulation techniques, which couples stochastic discrete events (for the coagulation and nucleation) with continuous processes (such as condensation, evaporation and precursor decomposition). We validate the MC method by comparison with the discrete-sectional method. The demanding simulation scenario incorporating all of the process discussed above poses special requirements not only on the MC method but also on the discrete-sectional method. We show the requirements (grid settings for the sectional methods, parameters for the MC simulations) for a correct description of the process.

In a second part, we discuss the application of the method on typical particle production processes for various materials (Fe, Ag, Cu, etc.). Special interest is given to the correct description of the nucleation process: several nucleation theories exist in the literature, which result in nucleation rates, which differ in several orders of magnitude. We propose a numerical methodology, which allows the identification of experimental conditions for the identification of the correct nucleation theory.

12AP.2**Modeling Smog Chamber Experiments: Forward and Inverse.**

NASER G. A. MAHFOUZ, Neil Donahue, *Carnegie Mellon University*

In environmental smog chambers, it is possible to isolate and study atmospheric particle chemistry and microphysics to illuminate how pollution contributes to the formation and growth of atmospheric aerosol particles. Oxidation of gas-phase precursors results in low-volatility products that condense onto growing aerosol particles. If the concentration of the formed low-volatility products is sufficiently high, they can also nucleate to form aerosol particles. Moreover, low-volatility products can be deposited onto the walls; likewise, suspended particles can be deposited onto the walls. Suspended particles coagulate inside the chamber resulting in bigger particles. Within a chamber, the dynamics of nucleation, condensation, coagulation, and deposition are all coupled; the purpose of this work is to separate these coupled processes to better model chamber dynamics, both forwardly simulating particle population changes and inversely determining the dynamics from available measurements. Where other models rely on ordinary differential equation (ODE) solvers, this work employs partial differential equation (PDE) solvers, since the underlying general dynamic equation (GDE) is a first-order hyperbolic PDE. Moreover, this work expands the space of uncertain parameters to account for more physical phenomena and measurements.

12AP.3**Latent Heat for Condensation and Coagulation During Nanocluster Growth.** HUAN YANG, Yannis Drossinos, Christopher Hogan Jr., *University of Minnesota*

Modelling of the growth rate of nanoclusters via monomer-cluster condensation or cluster-cluster coagulation is of importance in all aerosol systems where particles form from vapor phase precursors. An interesting feature of condensational and coagulative growth is that after a collision and binding event the internal energy of a newly formed cluster is higher than it would be at thermal equilibrium, i.e. condensation and coagulation events release heat. Typically, growth rate models are constructed either neglecting heat release (isothermal models) or assuming that the amount of heat released is equivalent to the bulk latent heat of evaporation. However, at the nanocluster scale, the heat released to a cluster is not necessarily equal to the bulk latent heat, and may depend non-monotonically on the number of atoms or monomers in the colliding clusters as well as the product cluster. In an effort to better understand heat release during cluster growth, we have developed a theory to calculate the heat release and latent heat for cluster growth as a function of the sizes (number of atoms or monomers) in the colliding clusters and the product cluster. We show that the latent heat, defined as the energy released to the surroundings because of a collision and binding event, and the internal energy increase associated with the binding event, are not equivalent at the nanoscale. The calculation approach depends upon (1) conservation of the total energy during collision between two clusters (or monomer and cluster), and (2) internal equilibration of the newly formed cluster in an NVE environment. We will present the derivation of the new theoretical expression and a case study using Molecular Dynamics simulations with a many-body, non-local Embedded-Atom Method potential for gold cluster growth.

12AP.4

Determination of Gas Phase Ion Structures of Locally Polar Homopolymers through High Resolution Ion Mobility Spectrometry-Mass Spectrometry. CARLOS LARRIBA-ANDALUZ, Xi Chen, *IUPUI*

The strong synergy arising from coupling two orthogonal analytical techniques such as ion mobility and mass spectrometry can be used to separate complex mixtures and determine structural information of analytes in the gas phase. A tandem study is performed using two systems with different gases and pressures to ascertain gas phase conformations of homopolymer ions polyethylene-glycol(PEG), polycaprolactone (PCL) and polydimethylsiloxane(PDMS). The studies of these three polymers are made using two very different IMS-MS systems and conditions albeit with the similarity that the mobilities calculated in both systems are directly related to the raw variables used. The first system is an ultra-high resolution ($R \sim 150-400$) 4m Drift Tube that operates at low pressure and He gas coupled to an in-house MS system. The second system is a high resolution ($R \sim 50-60$) DMA system that operates at atmospheric pressure in N₂ coupled to a commercial triple quadrupole Time of Flight system (ToF). Both systems use similar ESI sources to ionize the same analyte solutions in order to lower the amount of external variables that might affect the gas phase configurations.

Aside from the typical spherical and stretched configurations, intermediate configurations formed by a multiply charged globule and a "bead-on-a-string" appendix are confirmed for all three polymers. These intermediate configurations are shown to be ubiquitous for all charge states and masses present. For each charge state, configurations evolve in two distinctive patterns; an inverse evolution which occurs as an elementary charge attached to the polymer leaves the larger globule and incorporates itself into the appendage, and a forward evolution which reduces the globule without relinquishing a charge while leaving the appendix relatively constant. Forward evolutions are confirmed to form self-similar family shapes that transcend charge states for all polymers. Identical structural changes occur at the same mass over charge regardless of the system, gas or pressure strongly suggesting that conformations are only contingent on number of charges and chain length, and start arranging once the ion is at least partially ejected from the droplet, supporting a charge extrusion mechanism. The high resolution achieved with the drift tube allows many of the transitions to be completely resolved clearly for the first time where charge states "interweave". These transitions seem to extend to very high charge states and masses (up to the resolving power of the instrument and up to hundreds of kDa) without any observable difference in the family self-similar shapes. As such, the globule plus appendix structures present in PEG are confirmed for the other two polymers. Moreover, the transitions for PCL appear to be analogous to those of PEG while PDMS follows similar trends but with less sharp transitions. This is to be expected due to the increased steric hindrance caused by the methyl pendant groups. This study has implications in the study of the configurational space of more complex homopolymers and heteropolymers and other highly deformable particles.

12AP.5

Characterization of the Particle Wall Loss in the UCR Collapsible FEP-Teflon Chamber. CHEN LE, Don Collins, David R. Cocker III, *University of California, Riverside*

Understanding and correcting for particle wall-loss is critical for accurate determination of aerosol yield from environmental chamber studies. The most commonly applied methods for accounting for wall-loss are use of i) size-dependent corrections, ii) volume-averaged corrections, iii) inert tracer corrections, and iv) coagulation-corrected number-averaged corrections (Nah et al., 2017). Analysis of data from the UCR CE-CERT 90 m³ indoor chambers relies on corrections determined from the observed average rate of decay of the particle number concentration during the final few hours of each experiment when particle formation and growth are minimal. A size-independent correction has generally been assumed in part because it could explain the observed evolution of the size distribution of the late-experiment polydisperse aerosol. The magnitude of the loss rate and resulting correction is observed to vary from experiment to experiment and, especially because of the relatively long experimental time span (6~14 hours), the corrected aerosol yield is very sensitive to the average decay rate.

This study evaluates particle wall-loss characteristics in the CE-CERT chambers through a series of seed-only experiments in which one or more monodisperse ammonium sulfate particle modes were monitored over several hours. The average decay rate was found to increase with increasing particle size over the 50 nm to 400 nm diameter range examined. This pattern is believed to reflect a significant contribution of electrostatic loss of charged particles. This interpretation is further supported by the observation that the loss rate differed for injections of positively charged, negatively charged, and neutral particles. Size dependent particle wall-loss rates were evaluated as both a function of experimental time and as a function of the estimated ratio of the chamber wall surface area to the chamber volume (A/V). The sensitivity of particle wall-loss to chamber temperature was also investigated. In addition, a sensitivity analysis of SOA yields to corrections within the range of historical variations in daily particle wall-loss rates and a systematic comparison of the "size-dependent correction" and the "number-averaged correction" will be presented.

12AS.1

Variability Between High Time-Resolution PM Data from Regulatory Instruments: Implications for Low-cost Sensor Evaluations. KAROLINE BARKJOHN, Ian VonWald, Joann Rice, Robert Vanderpool, Tim Hanley, Andrea Clements, *U.S. EPA Office of Research and Development*

High time-resolution data (e.g., 1-minute to 1-hour) from low-cost air sensors, including PurpleAir sensors, is increasingly used to explore local air quality. The performance of air sensors is often assessed by comparison to a regulatory instrument; in most cases these monitors have been characterized by comparison to 24-hour integrated mass filter data and little is known about their performance at higher time-resolution. In this work, collocated Teledyne T640x and Grimm EDM 180 instruments measuring PM₁₀ and PM_{2.5} were compared for one year at a site in Durham, NC. During this period, gravimetric federal reference method (FRM) samples were collected daily for five months and three PurpleAir sensors were collocated for a separate three-month period. First, the error of the Grimm and T640x were determined versus the FRM on a 24-hour basis. Next, the relative measurement performance between the T640x and Grimm at various averaging intervals (1 minute to 24 hour) was compared and techniques aimed at improving the comparisons were explored. The results suggest these regulatory instruments can differ substantially at 24-hour averages and more at shorter averaging intervals. The large disagreement between monitors at short averaging intervals has implications for perceived sensor performance. This is demonstrated in our evaluation of PurpleAir sensors against both the Grimm and T640x over 1-minute to 24-hour averaging intervals. This work demonstrates that the selected comparison method may impact the calculated performance of an air sensor and highlights the limitations of comparing performance studies using different reference instruments. Future sensor evaluations should acknowledge the impacts of the comparison instrument type and should set reasonable expectations for sensor performance.

Disclaimer: 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.

12AS.2

Assessing the Accuracy and Reliability of Low-cost Particle Sensors for Quantifying Fine Particulate Matter. DAVID HAGAN, Eben Cross, Timothy Onasch, John Jayne, Douglas Worsnop, Jesse Kroll, *MIT*

The past several years has seen the emergence of many low-cost commercial devices for measuring particulate matter (PM). While these devices are beginning to see widespread use, little is known about their ability to accurately and repeatedly quantify fine particulate matter under realistic, dynamic conditions. Most commercially available devices can be classified as either photometers, integrating nephelometers, or optical particle counters; each of these technologies has strengths and weaknesses, but none measure mass directly. Thus, the extent to which they can be used to estimate particle mass concentration, the quantity on which most health-based assessments and PM regulations are based, is unclear. One of the key limitations for low-cost particle sensors is their inability to measure small particles (in the case of optical particle counters) and/or measure the underlying particle size distribution (in the case of nephelometers and photometers), which represent potential sources of error in PM mass measurements, especially in dynamic environments. Additionally, proprietary algorithms used by various sensor manufacturers to convert raw signal to concentration introduce additional challenges to such measurements. Here, we report the results of controlled laboratory experiments to explore the ability of several commonly-used low-cost (Alphasense OPC-N2, Alphasense OPC-N3, Plantower PMS5003, Particles Plus OEM, Handix POPS, GRIMM) and Federal Equivalent Method (FEM) particle sensors (Teledyne T640) to accurately quantify PM for particles across a range of sizes, optical properties, and relative humidities. Results will be presented comparing the ability of these devices to count and size particles relative to reference instruments (SMPS, CPC), as well as the relative strengths and weaknesses of the different instrument types (i.e. nephelometer vs. photometer vs OPC) for measuring particulate matter concentrations.

12AS.3

Characteristics of Ambient Ultrafine Particles Using a Combination of Low-Cost Sensors: Size Distributions and Volatility. MOLLY J. HAUGEN, Robert T. Nishida, Tyler T. Johnson, Anna K. Schroeder, Josh Hassim, Marc E.J. Stettler, Simone Hochgreb, Adam M Boies, *University of Cambridge*

Particle emissions are associated with a variety of health risks. However, the health risks are not currently well correlated to a particular particle metric. Health impacts may be related to the inhaled particle number, surface area, and mass, which may all have distinct health implications. Therefore, using laboratory grade instrumentation to measure these properties simultaneously is beneficial for air quality monitoring and epidemiological studies, albeit prohibitively expensive. Alternatively, low-cost instruments can monitor a range of ambient particle characteristics, and a deliberate combination of instruments provides more value than the sum of each individual instrument. Measurements made in the present study allows the first three moments of a particle size distribution to be determined, using low-cost sensors in a real-world urban environment.

The solid-carbon and volatile components of the ambient aerosol were determined using a catalytic stripper and duplicate low-cost sensors. A Naneos Partector (measuring lung-deposited surface area) measured occasions of purely volatile, nucleation mode aerosols which were not measured by the Alphasense UPM-S1 or micro-aethalometers (measuring active surface area and particle mass concentrations of the carbon component, respectively). The measured volatility and size components allows preliminary determination of the chemical composition and diameter, which can be correlated with particle origin. Video footage enabled correlations between emission spikes and vehicles typically associated with these emissions.

Particle size distributions were estimated using a combination of low-cost instruments over multiple days, including rush hour, midday, and minimal traffic activity. During high traffic periods, an ELPI+ particle classifier determined that particles in the size range 10-50 nm dominated the distribution, whereas during night-time, particle count was significantly reduced and larger particles (>100 nm) showed an increased contribution. The low-cost sensor measurements were consistent with these distributions. The study presented here provides a low-cost particle emission monitoring method that concurrently monitors various particle characteristics.

12AS.4

Ground- and Aerial-Based Platforms to Measure Aerosol Size Distributions: Spatiotemporal Variability, Vertical Profiles, and Near Source Sampling. SHANTANU JATHAR, Liam Lewane, Dylan Giardina, Shiva Tarun, Joshua Weller, Alex Lieberman, Kepler Worobec, Vance Payne, Tim Gordon, Gavin McMeeking, *Colorado State University*

The aerosol size distribution plays an important role in influencing the earth's radiative budget, cloud formation and properties, human health, and visibility. However, given the complexity, footprint, and cost of instrumentation, aerosol size distributions are not routinely measured, and data are generally restricted to short durations during intensive field campaigns. In this work, we leverage a light weight, low power, and lower cost optical particle counter called the POPS (portable optical particle spectrometer) manufactured by Handix Scientific to measure aerosol size distributions via ground- and aerial-based platforms. Our ground-based platform, the aPOPS (autonomous POPS), comprises a POPS, a solar-powered battery system, and an IoT (Internet of Things) module. The power system includes a 100 W photovoltaic solar panel charging a 36 Ah battery pack, which provides sufficient power for continuous year-round operation in Colorado. The IoT module is a cellular-based microcontroller that transmits aerosol size distribution data for up to 20 size bins to the Cloud every minute. A network of aPOPS systems will be deployed at four distinct locations over several weeks in Fort Collins, CO to investigate the spatial and temporal heterogeneity in aerosol size distributions within an urban environment. Our aerial-based platform, the UAV-POPS, comprises of a POPS, a CO₂ sensor, and an integrated IoT control board in an enclosure mounted on a hexacopter drone (Matrice 600). The IoT board processes and transmits the total aerosol number and volume concentrations and CO₂ data to the Cloud every twenty seconds. The UAV-POPS was deployed to measure vertical profiles in urban and suburban locations in Fort Collins, CO and will be deployed to measure aerosol emissions within prescribed burn plumes in the Colorado Front Range. Our work highlights the emerging area of using portable, lower cost sensors in environmental science research.

12AS.5

Six Years of Human and Machine Learning about Electrochemical Sensors. EBEN CROSS, David Hagan, Leah Williams, Douglas Worsnop, Jesse Kroll, John Jayne, *Aerodyne Research, Inc.*

Calibration methods for low-cost, electrochemical sensors generally fall into one of three categories: (1) Factory calibrations of batches of OEM sensors, (2) Laboratory 'chamber' calibrations, in which integrated sensor systems are exposed to known pollutant concentrations under a variety of temperature and humidity conditions, and (3) Ambient field co-location alongside reference monitoring equipment. There are advantages and disadvantages to each, but ultimately, the authenticity of a given calibration approach (or training data set) dictates the extent to which the sensor system can move from place to place and still provide reasonable quantification of the air pollution over time. In this presentation we will highlight some of the lessons that we've learned over the past ~ 6 years at Aerodyne and MIT working on integrated sensor systems, focusing on our work with electrochemical sensors. The duration of our ongoing projects (spanning months to years) and variety of environmental domains encountered (from wildfire, to near-road, to urban, to background) presents opportunities to further inform/refine/improve calibration model development moving forward. It's important to embrace the fact that all sensor systems are imperfect machines attempting to measure tiny perturbations in the concentration of a specific gas molecule in a complex and ever-changing ocean of air. We certainly have a lot more to learn in the years ahead, this presentation aims to focus some of those efforts.

12BA.1

Microbes Thrive in Clouds and Interact with Physico-chemical Processes: From Field Observations to Atmospheric Models. PIERRE AMATO, Barbara Ervens, Raphaelle Peguilhan, Laurent Deguillaume, Anne-Marie Delort, *ICCF, CNRS, Clermont Auvergne Université*

Cloud droplets offer aqueous environments to living airborne microorganisms in the atmosphere ($\sim 10^4$ cells/mL of condensed water), where they maintain metabolic activity. Using next generation sequencing approaches (16S and 18S rRNA genes sequencing, whole metagenomes and metatranscriptomes), we specified microbial biological functioning in cloud water samples collected from puy de Dôme summit's Atmospheric Observatory (1465 m asl; France). The results demonstrated a high taxonomic diversity in both prokaryotes and eukaryotes; the surviving organisms largely related to some abundant groups of bacteria affiliated with Alpha-, Beta- and Gamma-Proteobacteria, probably for a large fraction originating from vegetation. Metatranscriptomics specified their functioning and revealed intense interactions between cells and their direct environment in cloud water, with potential consequences for cloud chemical reactivity, including notably defense mechanisms against oxidants, cold and osmotic shocks, ions transport and binding, carbon and nitrogen compounds utilization (1). These, along with additional direct quantifications of biological aerosol mass, biological activity, biomarkers (ATP) and ice nucleation by biological particles in clouds and precipitation suggest a close interplay of biological, chemical, and microphysical processes. In order to estimate the amount of secondary biological mass that is formed by microbial processes in clouds, we combined the scarce data sets available for bacteria types and their activity in various ecosystems. We suggest that these processes might double primarily emitted bacteria in the atmosphere. In addition, we show that organic carbon processing by living microorganisms in clouds is probably negligible in terms of organic aerosol mass at the global scale. However, these processes might be important for the fate of specific chemical compounds. This research highlights the crucial need for experimental data for microbial aerosols, their diversity, dynamics and activity, and specifies directions for future investigations.

This research is currently funded by French Program ANR "Make Our Planet Great Again" MOBIDIC attributed to BE.

Reference:

[1] Amato P, Besaury L, Joly M, Penaud B, Deguillaume L, Delort A-M. 2019. Metatranscriptomic exploration of microbial functioning in clouds. *Sci Rep* 9:4383.

12BA.2

Real-time Monitoring and Modelling of Bioaerosols in Dublin, Ireland. Jose Manzano, Eoin McGillicuddy, Gavin Sewell, Paul Dowding, Matt Smith, Roland Sandra-Esteve, Dominique Baisnee, John Sodeau, DAVID O'CONNOR, *Technological University Dublin*

Primary Biological Aerosol Particles (PBAP) are an omnipresent component of atmospheric aerosols. PBAP consist of an assortment of entities of biological origin with pollen, bacteria and fungal spores among the most studied in the atmosphere.

PBAP has long been associated with health implications such as hayfever, COPD, asthma and aspergilliosis to name but a few. Allied to this PBAP also have the potential to act as cloud condensation nuclei or ice nuclei in cloud formation and thus have climatic inferences. Hence the need to study the concentration and composition of such particles is of interest to all.

However within Ireland little has been done with regard to the amounts or identity of biological particles in the literature. This work represents first sustained monitoring of PBAP in decades.

The work presented here has looked at both traditional (based on impactation on a filter and subsequent optical analysis) and newer real-time methodologies (utilizing fluorescence) for the monitoring of pollen and fungal spores at a site located in the heart of Dublin, Ireland. The sampling campaign utilized a Hirst volumetric trap, WIBS-4 and Japanese pollen counter to develop a seasonal cycle for the prevalence of pollen and fungal species in the Irish atmosphere. The real-time and traditional instrumentation were also compared and contrasted to evaluate whether real-time instrumentation was comparable to the currently most used technique (Hirst trap) around the world.

The traditional data in tandem with meteorological parameters, phenological data and source mapping were then used to formulate an Irish specific pollen model using several methods (multiple regression, random forest and neural networks). The incorporation of real-time pollen data into the models was then attempted with hope of increasing the accuracy, precision and timeliness of the forecasts.

12BA.3

Effect of Season and Environmental Parameters on Assemblages of Airborne Bacteria and Fungi in Mexico City. GEDIMINAS MAINELIS, Valdis Krumins, M. Hernandez, Jose Angeles, Victor Paramo-Figueroa, Martha Torres, Stephan Schwander, *Rutgers, The State University of New Jersey*

Earlier studies showed that exposure to ambient PM adversely affects protective human immune responses against *M. tuberculosis*, the causative agent of tuberculosis, possibly confounded by co-exposure to airborne microorganisms. Here we investigated the composition of airborne microbe assemblages in PM in a densely populated Iztapalapa municipality of Mexico City in 2016/2017.

Duplicate PM₁₀ samples were collected weekly for 24 hours at the height of 18 m using Impact Samplers (SKC Inc.) operated at 10 L/min. The accumulated microbial DNA was extracted and submitted to Molecular Research Laboratory (Shallowater, TX) for analysis of the 16S ribosomal RNA gene for prokaryotes and the internal transcribed spacer (ITS) region for fungi.

More than 3200 species of fungi in 150 orders (22 phyla) and more than 5000 species of bacteria belonging to 300 orders (50 phyla) were detected at highly varying relative abundances. More than 80% of bacterial communities were comprised of Actinobacteria, Proteobacteria, and Firmicutes. Forty percent of fungal reads belonged to orders identified as sooty mold, with *Cladosporium* spp. comprising ~40% of its genera; order Pleosporales, the majority species of which feed on decayed organic matter, comprised ~10% of reads; other major orders included Agaricales, Eurotiales, Polyporales, Hypocreales, and Xylariales (each >3%).

Principal coordinates analysis (PCoA) revealed seasonal effects (rainy vs. dry) and weather effects (rain/no rain during sampling) on the composition of the bacterial and fungal communities. Temperature, wind speed and direction, and relative humidity were weak predictors of microbial diversity. The ongoing data analysis is focusing on microbial diversity and richness indices and health-relevant species.

These preliminary data suggest that the makeup and abundance of microbes should be taken into account when analyzing exposures and potential health effects of outdoor PM.

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12BA.4

Complex Organic Particles from Terrestrial Sources as Ice Nucleators – More Than a Sum of Their Parts? ISABELLE STEINKE, Naruki Hiranuma, Ottmar Möhler, Susannah Burrows, *Pacific Northwest National Laboratory*

Vegetated areas or agricultural environments are potentially important sources for particles initiating the formation of ice crystals in clouds. In this work, we present results from lab-based studies investigating the ice nucleation properties of particles from leaf litter and agricultural soils at mixed-phase cloud conditions, i.e. at temperatures above 250 K. We also investigate the ice formation properties of individual organic components, e.g. plant-based lipids, which presumably contribute to the observed ice nucleation efficiencies. In most cases, however, we find that ambient particles tend to be significantly more ice-active than individual organic components.

12BA.5

Pollen Collection Campaign: Clustering and Classification Applications Utilizing a High-Spectral Resolution UV-LIF Instrument. BENJAMIN E. SWANSON, Samir Rezgui, J. Alex Huffman, *University of Denver, CO*

Biological aerosols are omnipresent in the atmosphere, and play a multitude of roles in both atmospheric processes and human health. Pollen, in particular, has a myriad of applications to human health, particularly in terms of allergenic response. Pollen detection, however, is frequently done either by a trained technician through visual microscopy. This, however, is time and cost-prohibitive for widespread usage to effectively map pollen allergies. As such, the ability to map real-time pollen populations in the atmosphere is relatively limited. Even recently developed real-time/commercial techniques have various hurdles, despite ultra-violet laser-induced fluorescence instrumentation being extremely power tools.

Here, we discuss our efforts over the previous pollination season (2018) to collaborate with the Denver Botanic Gardens and collect a large series of species in attempts to discover a good mechanism for pollen clustering and classification. Spectral data was collected from 34 individual species of pollen over the 2018 growing season and classified using three different clustering/classification algorithms: Hierarchical Agglomerative Clustering, KMeans Clustering, and Random Forest Classification. Data was collected on a previously developed inexpensive single-particle fluorescence spectrometer [1] that has been shown to have efficacy in pollen detection and separation [2]. The collected pollen was broken up into various delineation types, including pollination mechanism, allergenicity, and species, and classified using the Random Forest algorithm. Species were also classified along pollination season (spring, summer, fall) in order to produce a more realistic classification scenario. In these analyses, the random forest algorithm was able to classify pollen species at a general error rate of below 10%. We also show efforts to apply this analysis to ambient collections of pollen. In efforts towards successful classification in developing an inexpensive pollen sensor, we also demonstrate initial efforts in source-reduction and the effects removing any one piece of data would have on the overall classification efficacy.

References:

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12CA.1**Spatio-temporal Trends and Source Apportionment of PM_{2.5} Organic Carbon Thermal Fractions (OC_x) across the Los Angeles Basin.**

EHSAN SOLEIMANIAN, Amirhosein Mousavi, Sina Taghvaei, Mohammad Sowlat, Sina Hasheminassab, Andrea Polidori, Constantinos Sioutas, *University of Southern California*

The main objective of this study was to identify and quantify the sources of organic carbon (OC) and its thermal fractions (OC_x) across the Los Angeles Basin in five sampling sites, including West Long Beach, Anaheim, central Los Angeles (CELA), Rubidoux, and Fontana from July 2012 to June 2013. Total OC and OC volatility fractions (OC₂-OC₄), measured by thermal optical analysis as part of the fourth Multiple Air Toxics Exposure Study (MATES IV), gaseous pollutants, and particulates source tracers were used as the input data to Positive Matrix Factorization (PMF) receptor model. Vehicular emissions, secondary organic aerosols (SOA), and biomass burning were identified as the three major sources of OC and OC_x across the sampling locations with a corresponding average contribution of 56±9%, 42±7%, and 5±3% to total OC, respectively. In addition, traffic contributed as the major source to OC₂ and OC₃ at the upwind sites of West Long Beach and CELA with the corresponding contribution of 79% and 60% to OC₂, and 64% and 53% to OC₃, respectively. On the other hand, SOA was the dominant contributor to OC₄, especially in the downwind receptor sites with the corresponding contributions of 56% and 66% in Fontana and Rubidoux, respectively. Vehicular emissions and biomass burning were more significant during winter phase mainly due to the atmosphere stability and lower mixing height, while SOA contribution to total OC increased during warm phase as a result of higher photochemical activities. Results from this study provided insights regarding the sources and spatio-temporal variations of OC and OC_x concentrations in PM_{2.5} across the Los Angeles Basin which can be used as an indicator of the extent of human exposure to primary and secondary aerosols.

12CA.2**Biases in Quantifying Light Absorption Enhancement for Coated Black Carbon Aerosol Using a Thermodenuder.**

NISHIT SHETTY, Apoorva Pandey, Wei Min Hao, Stephen Baker, Rajan K. Chakrabarty, *Washington University in St. Louis*

Recent observational findings suggest black carbon (BC) aerosol to primarily exist in a mixed state with organic compounds (OC). Visually, the mixed OC exists as shell coatings on BC cores (aggregates). The magnitude of light absorbed by BC aerosol gets enhanced upon internal mixing with non-absorbing and weakly absorbing OC. A thermodenuder is a widely used instrument to study the enhancement (E_{abs}) in BC light absorption. It operates by heating the aerosol stream to vaporize condensed organics followed by removal of the generated gas phase OC using activated carbon denuders. The magnitude of E_{abs} can be determined by quantifying aerosol absorption coefficients before and after thermodenuding the particle stream. Values of E_{abs} obtained using a thermodenuder may suffer from biases due to incomplete stripping of OC coatings and/or thermophoretic losses of particles inside the instrument. We performed experiments to investigate these biases as a function of the thermodenuding temperature for coated BC particles generated from biomass burning. The amount of BC and OC present post-thermodenuding was quantified using the IMPROVE thermal/optical reflectance method. In addition to E_{abs} , change in optical properties such as the single scattering albedo and Absorption Ångström Exponents were also measured with varying temperature. This presentation will conclude by summarizing the potential impacts of thermodenuder biases on BC light absorption enhancements, explain recent field observations, and provide recommendations for future research making use of this instrument.

12CA.3

Development of a Universal Correction Algorithm for Filter-Based Absorption Photometers. HANYANG LI, Gavin McMeeking, Andrew May, *The Ohio State University*

Light-absorbing atmospheric particles directly affect the Earth's energy budget by absorbing solar radiation. There are various measurement approaches to quantify light absorption (B_{abs}) *in situ*, but our interest here is filter-based absorption photometers due to their near-ubiquity in monitoring networks around the globe. One challenge with filter-based absorption photometers is that biases can arise due to the presence of the filter. Consequently, various correction algorithms exist to minimize these biases; some are applicable to the Particle Soot Absorption Photometer (PSAP), while others are applicable to the Aethalometer (AETH).

We conducted laboratory experiments to investigate aerosol emissions from simulated wildfires, including three filter-based absorption photometers: an AETH, a Continuous Light Absorption Photometer (CLAP) and a Tricolor Absorption Photometer (TAP). Our analysis of the B_{abs} indicates that even when the correction algorithms are applied, issues remain such as: 1). Corrected filter-based B_{abs} may remain biased relative to a reference value of B_{abs} ; 2). Derived products (such as absorption Ångström exponents) may differ based on the implemented correction algorithm; 3). The applicability of previous correction algorithms to more recently developed instruments (e.g., CLAP and TAP) remains ambiguous.

Consequently, we have developed a "universal" correction algorithm across multiple wavelengths that is applicable to any filter-based absorption photometer by combining observed filter-based B_{abs} with scattering coefficient (e.g., from a co-located nephelometer) and reference B_{abs} (e.g., from a co-located photoacoustic instrument). The algorithm can even extend to situations where a filter-based absorption photometer is operated without a co-located nephelometer. We have applied the algorithm to both laboratory data and ambient data (from the DOE ARM Southern Great Plains user facility). Our algorithm results in very good agreement between filter-based and *in situ* B_{abs} for both source-generated biomass burning smoke and ambient aerosols.

12CA.4

Prediction of Black Carbon Mass Absorption Cross Section: Effects of Particle Morphology and Refractive Index. FENGSHAN LIU, Jerome Yon, Andrés Fuentes, Joel Corbin, Prem Lobo, Gregory Smallwood, *National Research Council Canada*

Mass absorption cross section (MAC) is an important parameter in optically based methods to convert the measured black carbon (BC) absorption coefficient to BC mass concentration. The commonly used MAC values in instrumentation are based on limited measurements from different BC emission sources of different particle morphology and particle size. It is known that the measured MAC values display a fairly large deviations from one measurement to another and it is not entirely clear if such deviations are due to the different microstructure (maturity) of BC particles, different measurement methods, or different BC particle morphology and size. Several experimental measurements have showed that the measured MAC exhibits fairly large size dependence.

In this study, MAC of BC aggregates of different morphology (primary particle diameter, fractal dimension, primary particle overlapping and necking) was numerically investigated using GMM and DDA by assuming different refractive indices in the visible and near infrared. The results show that the predicted MAC values of typical BC aggregates emitted from combustion systems display deviations on the order of 20% due to variation in morphology. The refractive index (microstructure of BC) has a stronger influence on the predicted MAC. Moreover, the effect of BC particle morphology on the predicted MAC is dependent on the assumed refractive index. The results can be interpreted by the multiple scattering effects among primary particles within a BC aggregate. The results suggest that the uncertainty of MAC of BC particles emitted from different sources is likely to be higher than 10%. This uncertainty in MAC will propagate to the measured BC mass concentration inferred from the measured BC absorption coefficient.

12CA.5**Quantifying the Thickness of Volatile Particle Coatings.**

OGOCHUKWU ENEKWIZU, Ali Hasani, Mary McGuinness, Alexei Khalizov, *New Jersey Institute of Technology*

The changes in morphology and mixing state of soot aggregates strongly influence their optical properties. Our previous research has shown that preferential condensation of vapors in the junctions between monomer spheres that compose soot aggregates drives the restructuring of those aggregates. However, establishing a relationship between the degree of restructuring and amount of condensate proved to be a challenge in the case of intermediate volatility vapors due to partial condensate evaporation during aerosol transit from the coating chamber to the detection point. To address this challenge, we built a custom electrostatic precipitator that could be placed at any position after the exit from the coating chamber. The precipitator was calibrated against spherical particles of known sizes and then used to determine the growth profiles of the soot aggregates that were exposed to different amounts of condensable vapor. The amount of condensate lost as a function of transit time was measured as well by varying the distance from the coating chamber to the precipitator. Additionally, for experimental measurements performed using spherical particles, a comparison against the results of a simple aerosol condensation/evaporation model was performed. The results of this study confirm the validity of our previous conclusions regarding the role of capillary condensation in the restructuring of soot aggregates. The implications of our findings on the representation of soot morphology and mixing state in global climate models will be discussed.

Keywords: soot, morphology, mixing state, supersaturation, volatility, restructuring

12IS.1**Modeling Indoor Surface Chemistry Using Kinetic Multilayer Models.**

Pascale Lakey, Glenn Morrison, James Mattila, Youngbo Won, Krista Parry, Michael von Domaros, Douglas Tobias, Donghyun Rim, Jonathan Abbatt, Delphine K. Farmer, MANABU SHIRAIWA, *University of California, Irvine*

Kinetic multilayer models were used to gain a better understanding of two different important indoor chemical systems; (1) the reactions of ozone with clothing and the formation of squalene ozonolysis products, (2) chemical processes in an indoor boundary layer and indoor surfaces. Both models treat chemical reactions and diffusion as well as adsorption and desorption to a surface.

The clothing model was able to reproduce measurements of carbonyls formed when ozone reacted with soiled clothing. Several parameters were constrained by molecular dynamic simulations. We demonstrated that clothing protects underlying skin from ozone and that soiled clothing can lead to carbonyl concentrations increasing to ppb levels depending on air exchange rates. Model outputs were inputted into a computational fluid dynamic model to estimate the distribution of ozone and squalene ozonolysis products throughout a room.

An indoor boundary layer model was developed to better understand the concentration gradient of OH radicals near indoor surfaces. It was shown that by including the chemistry of ozone with terpenes in the boundary layer, the OH uptake rate to surfaces was larger than would be predicted by traditional models. Factors which affected the OH uptake rate included the O₃ uptake coefficient and the degree of turbulence within the room. In addition, we simulated the formation and loss of species in the gas phase upon floor-bleaching as measured during the HomeChem campaign. The model included a boundary layer next to the bleach and reactions occurred in the aqueous bleach, in the gas phase and on particle and room surfaces. The model was able to reproduce the loss of ammonia and the formation of chloramines.

12IS.2

Multiphase Reaction Mechanisms of Criegee Intermediates in Indoor Environments. KEVIN WILSON, *Lawrence Berkeley National Laboratory*

Developing molecular predictions of how oxidants react with unsaturated hydrocarbons in organic aerosols and at indoor surfaces remains a considerable challenge. Recent work has focused on developing predictive O₃ and OH multiphase reaction mechanisms of simple alkene surfaces (e.g. squalene). Our goal is to understand how individual elementary reaction steps of radical and Criegee intermediates (CI) in turn drive macroscopic changes at an interface (i.e. chemical erosion). To do this we combine kinetic simulations with vacuum ultraviolet (VUV) photoionization aerosol mass spectrometry and nanoparticle X-ray photoelectron and absorption spectroscopies. I will describe how condensed phase CI's react with trace gases such as H₂O and SO₂ to drive both chemical erosion and the production of reactive gas phase species. I will highlight key differences and similarities between heterogeneous reactions of OH vs. O₃ at squalene interfaces.

12IS.3

Formation of Isocyanic Acid from the Heterogeneous Ozonolysis of Tobacco Smoke Deposited onto Indoor Surfaces. CHRISTOPHER LIM, Jonathan Abbatt, *University of Toronto, Canada*

Indoor air pollution can lead to significant exposures to toxic compounds (e.g., harmful gases and particulate matter), especially for populations who spend a majority of their time indoors. Despite the importance of indoor air, chemical transformations indoors are relatively understudied compared to those that occur outdoors. One defining feature of the indoor environment is the large amount of surface area available (typically orders of magnitude higher than the outdoors) for semivolatile compounds to deposit onto. In addition to dermal exposure to occupants, compounds deposited onto surfaces can continue to react through heterogeneous reactions with atmospheric oxidants over long timescales (days to weeks) since they are less subject to removal by building air exchange. In this work we focus on the ozonolysis of tobacco smoke, an important source of indoor air pollution, deposited onto a variety of indoor surface proxies and use an acetate ion time-of-flight chemical ionization mass spectrometer (CIMS) to detect gas-phase products volatilized from the surface. Over a wide range of environmental conditions, isocyanic acid (HNCO) is detected as a major product, showing the capability of surface reactions to be an additional source of exposure to toxic compounds indoors.

12IS.4

Change in Reactivity of Organic Aerosols toward Heterogeneous OH Oxidation over Reaction Time. Man Mei Chim, Christopher Lim, Jesse Kroll, MAN NIN CHAN, *The Chinese University of Hong Kong*

Oxidation initiated at or near a particle surface by gas-phase oxidants can continuously change the composition and properties of organic particles, which in turn alter the heterogeneous reactivity over time. However, chemical transformation of organic particles by heterogeneous oxidation is typically described by a single kinetic parameter (effective OH uptake coefficient, γ_{eff}), which implicitly assumes the reactivity does not change significantly over their atmospheric lifetimes. Using time-resolved particle composition and size data measured in an environmental chamber, we find that the heterogeneous reactivity of citric acid toward gas-phase OH radicals continuously decreases over reaction time and slows down by 16% after oxidation equivalent to about 2 days of OH exposure. This could be explained by consumption of citric acid, and its concentration at the particle surface drops due to OH oxidation and the formation of reaction products during oxidation. This lowers the reactive collision probability between citric acid and gas-phase OH radicals at the gas-particle interface, leading to a smaller overall reactivity. The results suggest that the use of a single kinetic parameter could overpredict the heterogeneous OH oxidative loss rate of citric acid and other organic compounds over their atmospheric time scales.

12IS.5

Methods for the Quantification and Identification of Alkenes on Indoor Surfaces. BENJAMIN DEMING, Paul Ziemann, *University of Colorado*

The deposition and accumulation of aerosols and gases to surfaces can lead to the formation of surface films. These films are believed to be ubiquitous indoors, where they can act as sinks for semi-volatile organic compounds (SVOCs), reactors for condensed-phase reactions, sites of heterogeneous gas-condensed-phase reactions, and exposure routes for human health impacts. The majority of studies investigating these films have been performed on impermeable surfaces, typically window glass. Painted surfaces, which tend to dominate by surface area, potentially differ from glass in several important ways, and are therefore an understudied aspect of indoor environments. The presence of unsaturated compounds within these films can result in secondary emissions from surfaces through ozonolysis reactions. To explore these areas of interest we characterized a method for quantitatively sampling the low-volatility, organic portion of a surface film using a surface wipe and developed a spectrophotometric method for quantifying nanomole quantities of alkenes. Samples were also derivatized, adding a readily ionizable group to non-conjugated double bonds, allowing for identification by positive-mode ESI-MS. Samples from neighboring glass and painted surfaces were collected from a variety of locations, including a classroom, graduate student offices, a bowling alley, a gym, and more. Filter and surface samples taken concurrently allowed the ambient aerosol to be compared with nearby surface films. To investigate the effect of cooking on nearby surface concentrations we pan-fried three different cooking oils at high temperatures and analyzed the double bond content of the raw oil, cooked oil, and nearby surfaces. Samples taken during the indoor air field studies HOMEChem and ATHLETIC were also analyzed. The results from this work should be useful to the modeling of indoor environments and help assess the importance of surfaces to indoor chemistry.

13AC.1

A Diversity and Distribution of Organic Aerosol Functional Groups across Multiple Sites and Seasons. JENNA DITTO, Taekyu Joo, Jonathan Slade, Paul Shepson, Nga Lee Ng, Drew Gentner, *Yale University*

Highly functionalized organic compounds are known to be a major component of secondary organic aerosol in urban, downwind, and remote environments. However, these complex mixtures of compounds are understudied at the molecular level, and the impact of changes in the molecular-level composition of aerosol mixtures on air quality is often poorly understood. Characterizing the functional group distribution of organic aerosol (OA) can help constrain reaction pathways and products in the atmosphere, and ultimately improve our understanding of the health and environmental impacts of OA. Here, we leverage liquid chromatography with electrospray ionization and quadrupole time-of-flight tandem mass spectrometry (LC-ESI-MS/MS) to characterize the molecular-level elemental and structural characteristics of OA. A non-targeted screening of OA functional groups from a forest, from a major US city, and from aged urban outflow shows a diverse range of oxygen-, nitrogen, and sulfur-containing structures. We observe important contributions from hydroxyl groups (~25-30% relative prevalence), carboxylic acids (~5-20%), and esters (~7-10%), along with a range of other functional groups with smaller but persistent contributions across ambient locations, including amines, organonitrates, and organosulfates. We compare the structural features present in functionalized OA across time of day, season, and location. Urban summertime data show a greater proportion of hydroxyl groups, carboxylic acids, carbonyls, and non-aromatic rings relative to the winter, while we observe an increased proportion of amines and aromatic rings at the same site in winter. Comparing urban and aged urban outflow functional group distributions, we observe an increased contribution from carboxylic acids, carbonyls, and amines at the urban site, and an increased contribution of esters in urban outflow. Finally, we use these results to identify key characteristics of OA functional group distribution and associated implications for OA properties and impacts.

13AC.2

Characterization of Organics in Cloud Water: Measurements from the Present Day and from Decades Past. SARA LANCE, Christopher Lawrence, Jie Zhang, Qi Zhang, Liaquat Husain, Dan Kelting, Elizabeth Yerger, Hunter Favreau, James Schwab, Paul Casson, Richard Brandt, *University at Albany, SUNY*

An emerging trend of increasing water soluble organic carbon (WSOC) has been observed in cloud water over the past decade at Whiteface Mountain (WFM) in Upstate New York. This trend is correlated with a growing inorganic ion imbalance and a growing fraction of ammonium, which in recent years has begun to surpass sulfate and nitrate combined. Altogether, these independent observations suggest that uncharacterized anions, which now make up a significant fraction of the cloud water composition in the northeastern U.S., are comprised of organic compounds. The driving factors behind such a striking increase in cloud water WSOC and potential impacts on secondary organic aerosol mass loadings are not clear, highlighting a need to better characterize the chemical makeup of the organic constituents in cloud water. Low molecular weight organic acids have now been added to the routine suite of cloud water chemical measurements at WFM, and we report on our first year of organic acid observations. While including eight organic acids that are typically found to be most abundant does significantly improve the anion deficiency, on average 28% of the anions remain uncharacterized. The organic component is further characterized using a high resolution time-of-flight aerosol mass spectrometer. Comparisons of recent and historical organic observations at WFM are presented.

13AC.3

Linking Organic and Sulfate Concentrations to the Annual Phytoplankton Bloom Cycle in the North Atlantic. GEORGES SALIBA, Chia-Li Chen, Savannah Lewis, Lynn Russell, Derek Coffman, Patricia Quinn, Lucia Upchurch, Timothy Bates, Michael Behrenfeld, *Scripps Institution of Oceanography*

Organic and sulfate particles are ubiquitous above oceans and dominate aerosol number concentrations. These particles have sizes often larger than the critical activation diameter and hence constitute a large fraction of cloud condensation nuclei. Strong seasonal variations in organic and sulfate concentrations have been associated with phytoplankton blooms, however, the link between seawater biology and chemical composition of atmospheric aerosol is still not clear. In this study, we present results from the unprecedented coverage of atmospheric and ocean parameters from four North Atlantic Aerosols and Marine Ecosystems Study (NAAMES) campaigns to investigate the variability in chemical composition of aerosol, on hourly and seasonal timescales, using a time-of-flight aerosol mass spectrometer. Organic concentrations varied significantly from a high of $0.4 \pm 0.2 \mu\text{g}/\text{m}^3$ (during late spring biomass climax) to a low of $0.07 \pm 0.04 \mu\text{g}/\text{m}^3$ (during winter biomass minimum). Moreover, median seasonal organic concentrations correlated strongly with median seasonal chlorophyll concentrations ($r > 0.9$, $p < 0.05$), suggesting organic particles in the marine boundary layer (MBL) are mainly of primary origin and to a lesser extent formed by secondary processes. Sulfate concentrations also showed a seasonal dependence; sulfate was highest during early spring (biomass accumulation transition) with a mean of $0.3 \pm 0.2 \mu\text{g}/\text{m}^3$ and lowest during winter (biomass minimum), $0.07 \pm 0.07 \mu\text{g}/\text{m}^3$. We will further investigate the sources and variability of both primary and secondary organic and sulfate particles in the MBL using methane sulfonic acid as a tracer of secondary organic aerosol and using elemental composition from high-resolution measurements.

13AC.4

Aerosol Precursors from Agricultural Emissions. PHILIP SILVA, *USDA - Agricultural Research Service*

Aerosol influences on the environment from agriculture are usually considered to be dominated by coarse mode dust with some secondary component in the fine mode from the impact of ammonia emissions. However, agricultural emissions include many reactive volatile organic compounds that potentially contribute to secondary aerosols as well. Emissions inventories are more uncertain regarding area sources like agriculture compared to mobile and point sources. In a number of locations, measured ammonia is either significantly higher or lower than modeling would predict and most reactive organic compounds are not adequately accounted for. Is this because different management practices contribute emissions different than specified inventory values? Are there missing sources in emissions inventories? We have performed field sampling experiments at poultry, dairy, and a hog farms to find answers to these questions. We will show evidence from field work that ammonia and volatile organic compounds react close to source to produce aerosol and discuss potential formation mechanisms. Data suggest that agricultural emissions may be underestimated as a source for new particulate matter in rural areas and that emissions inventories and air quality models may be missing important information.

13AC.5

Urban Pollution Greatly Enhances Formation of Natural Aerosols over the Pristine Amazon. MANISHKUMAR SHRIVASTAVA, Meinrat O. Andreae, Paulo Artaxo, Henrique Barbosa, Larry Berg, Joel Brito, Joseph Ching, Richard Easter, Jiwen Fan, Jerome Fast, Marianne Glasius, Allen Goldstein, Eliane Gomes, Helber Gomes, Dasa Gu, Alex Guenther, Shantanu Jathar, Saewung Kim, Sijia Lou, Scot T. Martin, Alla Zelenyuk, Rahul Zaveri, John Shilling, Joel A. Thornton, et al., *Pacific Northwest National Laboratory*

Understanding how anthropogenic emissions have modified natural biogenic secondary organic aerosol (SOA) formation constitutes one of the largest uncertainties in our understanding of the radiative forcing of climate. Due to ubiquitous influence of anthropogenic emissions over most terrestrial locations in the Northern Hemisphere, it is difficult to establish baseline biogenic SOA formation i.e. biogenic SOA that would be formed in the absence of anthropogenic perturbations. The vast Amazon rainforest during its wet season is one of the few remaining places on Earth where atmospheric chemistry transitions between preindustrial-like and present-day polluted conditions and serves as a unique natural laboratory to study anthropogenic-biogenic interactions. We develop insights from several laboratory measurements to simulate SOA formation in the wet-season Amazon using a high-resolution regional model (at 2 km grid spacing) and develop mechanistic insights about the role of anthropogenic emissions in biogenic SOA formation. We perform model simulations using the community regional Weather Research and Forecasting Model coupled to chemistry (WRF-Chem) at cloud-, chemistry-, and emissions-resolving scales i.e. at 2 km grid spacing. Sensitivity simulations that turn the urban emissions on/off are performed to quantify the impacts of anthropogenic-biogenic interactions on SOA formation. We evaluate WRF-Chem simulations using aircraft-based field measurements of SOA during the Green Ocean Amazon (GoAmazon 2014/5) field campaign. Our results show that urban emissions increase concentrations of nitrogen-oxides (NO_x), which cause increase in oxidant (ozone and OH radical) concentrations within the otherwise pristine Amazon. Increased oxidant concentrations catalyzed by NO_x substantially increase reactions of forest organic carbon, emitted as volatile organic compounds (VOCs include isoprene, monoterpene and sesquiterpene compound classes), and thereby enhance biogenic SOA formation by 60-200% on average in plume-influence regions. Model simulated enhancements agree with those observed by the aircraft which rapidly and concomitantly measures organic aerosols in background and plume-influenced locations using the Aerosol Mass Spectrometer (AMS). Our results provide a clear picture of how anthropogenic emissions might have substantially enhanced natural biogenic SOA formation since preindustrial times on Earth.

13AP.1

Spherical Particle Absorption over a Broad Range of Imaginary Refractive Index. CHRISTOPHER SORENSEN, Justin Maughan, Hans Moosmuller, *Kansas State University*

We present studies of the optical absorption cross section for homogeneous spheres of radius R interacting with light of wavelength λ as calculated with the Mie equations. Four regimes of behavior are disclosed: the Rayleigh Regime, the Geometric Regime, the Reflection Regime, and a Crossover Regime. Two parameters govern these regimes, the imaginary part of the refractive index, κ , and the product of κ with the sphere size parameter kR where $k = 2\pi/\lambda$, i.e. κR . Simple, approximate functionalities on κ , k , sphere volume and projected geometric cross section are derived for these regimes. Interesting aspects of our observations include: Rayleigh absorption can apply to all particle sizes, Fresnel reflection can occur for sub-wavelength spheres, and while κ is the agent of absorption, large κ can increase scattering to the detriment of absorption.

13AP.2

Estimating Uncertainties in Refractive Index Retrievals from Optical Closure Calculations using Full Aerosol Size Distributions. ALEXANDER FRIE, Roya Bahreini, *University of California, Riverside*

The refractive index (m) is the fundamental descriptor of a material's optical properties. For aerosols, m can be used to calculate their direct radiative effect within the atmosphere. Spherical aerosol refractive indices are commonly calculated using different optical closure methods, where the observed optical properties are compared to those predicted using Mie theory for different m values. One method uses a series of monodisperse aerosol populations and associated optical measurements to calculate m (*Size Selected*), and another uses the bulk size distribution and associated optical measurements (*Full Distribution*). Due to the time needed to switch between multiple diameters, the *Size Selected* method has limited field and laboratory applications if aerosol properties are highly dynamic. Alternatively, *Full Distribution* measurements are faster and have potential field applications. Given this, it is important to understand the uncertainties associated with the *Full Distribution* retrievals. Due to the complexity of Mie theory, and its computational expense, propagation of measurement uncertainties through the m retrievals has been difficult. Despite this, constraining the uncertainty in m retrievals is essential as it may change depending on the m value, observational uncertainties, and the aerosol size distribution. Here a pseudo-Monte Carlo tool is developed which propagates instrumental uncertainties through the m calculations via simulating multiple possible "true" m values, perturbing size distribution and optical characteristics with instrumental uncertainties, and recalculating m using the perturbed values. Repeating these calculations a large number of times yields a probability distribution of m values which could have yielded the originally retrieved m , indicating its uncertainty range. Results from this tool are demonstrated using seven representative aerosol size distributions over a series of m values and a series of uncertainty conditions. These simulations reveal the importance of considering aerosol size distribution, m , and instrumental uncertainties when reporting aerosol m values.

13AP.3

Surface Tensions of Picoliter Droplets with Sub-Millisecond Surface Age. BRYAN R. BZDEK, Rachael E.H. Miles, Michael Glerum, Hallie Boyer, Jim Walker, Jonathan P. Reid, Cari Dutcher, *University of Bristol*

Aerosols are key components of the atmosphere and play important roles in many industrial processes. Because aerosol particles have high surface-to-volume ratios, their surface properties are especially important to their reactivity and cloud droplet forming potential. However, direct measurement of the surface properties of aerosol particles is challenging. In this work, we describe a new approach to measure the surface tension of picoliter volume droplets with surface age <1 ms by resolving their dynamic oscillations in shape immediately after ejection from a microdroplet dispenser. Droplet shape oscillations are monitored by highly time resolved (500 ns) stroboscopic imaging, and droplet surface tension is accurately retrieved across a wide range of droplet sizes (10-25 μm radius) and surface ages (down to $\sim 100 \mu\text{s}$). The approach is validated for droplets containing sodium chloride, glutaric acid, and water. Experimental results from the microdroplet dispenser approach are compared to complementary measurements of the surface tension of 5-10 μm radius droplets with aged surfaces using a holographic optical tweezers approach and predictions of surface tension using a statistical thermodynamic model. The approach was then applied to study surfactant partitioning in freshly produced picoliter droplets on microsecond timescales. These approaches combined allow investigation of droplet surface tension across a wide range of droplet sizes, compositions, and surface ages.

13AP.4

Optical Properties and Q-space Study of Fractal-like Soot Aggregates from Coal Combustion Based on 3-D Electron Tomographic Reconstruction. CHENCHONG ZHANG, William Heinson, Jingkun Jiang, Rajan K. Chakrabarty, *Washington University in St. Louis*

Soot aggregates constitute the major fraction of particulate matter emitted from anthropogenic sources. Freshly emitted soot particles have complex fractal-like morphologies that can significantly influence the particles' microphysical and optical properties, thereby impacting the earth's radiative forcing.

Diffusion limited cluster-cluster aggregation (DLCA) has been considered as a high-fidelity simulation of soot aggregates generation process. The most optical and morphological studies of fractal-like soot particles are based on DLCA aggregates. However, there are few studies accurately parameterize soot aggregates' morphology and quantitatively evaluating their spectral radiative properties based on their real shape. In this study, we detect the detailed three-dimensional (3-D) structure of aggregates by using electron tomography technique. To compensate for 'the missing wedge', an inherent defect of limited-angle projection images, we incorporate total variation minimization in addition to traditional weighted back projection approach. The reconstructed soot particle models precisely capture detailed morphological information about the aggregates, for example, the exact shapes of primary particles and the necking between monomers. Next, we calculate the Fourier transform of the density auto-correlation function of the voxels (also known as the particle structure factor) to accurately characterize the fractal morphology of the reconstructed particles. Our goal is to validate the conventional view that combustion-generated fractal aggregates formed via DLCA, have a universal mass fractal dimension of 1.8. Finally, we conclude this work by applying the discrete-dipole approximation on reconstructed aggregate models to derive their spectral optical properties, including scattering and absorption cross-sections, and asymmetry and Stokes parameters.

13AP.5

Aerodynamic Resuspension of RDX Trace Particles by Planar Impinging Air Jet. KALYAN KOTTAPALLI, Harikrishnan Murali, Guanyu Song, Igor Novosselov, *University of Washington*

Trace residues of illicit substances and biological contamination of the surfaces remain accessible for long times because of their low volatility. Though the non-contact surface sampling has been demonstrated, the resuspension rates for an extended range of particle/surface systems are needed. Aerodynamic particle resuspension is a function of many parameters, such as particle size, morphology, surface properties, environmental conditions, and wall jet properties. We present the data and analysis of the removal rates of Trimethylenetrinitramine (RDX) resulted from an impinging flat jet as a function of wall shear stress. Samples are prepared by dry transfer method on the glass surface and interrogated under various flow conditions and exposure times. The samples are examined optically and binned by their visible area. The resuspension data for 6-30 μm particles from the impinging jet experiment are correlated with forces acting on the particles from Computational Fluid Dynamics (CFD) modeling as a function of wall shear stress showing a direct correlation with the particle removal rates. The removal efficiency of RDX from glass increases by 8-14 % with an increase in the flow exposure time.

13AS.1

Applicability of Different Type Particulate Matter Sensors to Urban Air Quality Measurements. JOEL KUULA, Heino Kuuluvainen, Topi Rönkkö, Jarkko Niemi, Erkka Saukko, Harri Portin, Minna Aurela, Sanna Saarikoski, Rostedt Antti, Hilikka Timonen, *Finnish Meteorological Institute*

Dense monitoring networks are required for detailed spatiotemporal characterization of urban air quality. Conventional instrumentation is often conceived as bulky and expensive and hence inadequate to be used in monitoring networks. Prospective alternatives for these instruments are small sized and low-cost sensors specifically designed for network applications. However, as urban air composes of complex mixture of particles with different physical properties, it remains indefinite how sensors with reduced capabilities are best utilized in urban air quality monitoring.

Applicability of two different type particulate matter measurement techniques to urban air quality measurements were studied at a street canyon site in Helsinki, Finland. The measurement station was located in the immediate vicinity of a busy street which consequently highlighted vehicular exhaust emissions. However, long-range transported and street dust episodes were also observed. The tested sensors were a custom build optical Prototype Aerosol Sensor (PAS, utilized Shinyei PPD60PV and PPD42NS sensor modules as its detection units) and three commercial diffusion charging-based sensors (Pegasor AQ Urban, DiSCmini and Partector). Sensors were compared against Tapered Element Oscillating Microbalance (TEOM, PM_{2.5} and PM_{2.5-10}) and Differential Mobility Particle Sizer (DMPS, lung deposited surface area) reference instruments.

The results showed that the optical sensor was not able to measure ultrafine particles emitted from vehicular exhaust emissions due to their small size (< 0.5 μm). However, it was able to observe local street dust and long-range transported particles with good accuracy. Diffusion-charging sensors were well-suited for measuring of vehicular emissions. These results highlight that supplemental sensor networks are best leveraged when the used measurement technique is chosen according to the features and limitations set by the specific environment. Additionally, the density of the measurement points should be determined according to the locality of the pollution sources as particles originating from longer distances (i.e. long-range transported) show much smaller city-scale spatial variability than e.g. local traffic.

13AS.2

Evaluation of a New Low-Cost Particle Sensor as an IoT Device for Outdoor Particulate Matter Monitoring. ANDREW METCALF, Christopher Post, John Pearce, Austin Green, Nilima Sarwar, Elena Mikhailova, Michael Cope, *Clemson University*

Low-cost particle sensors provide an opportunity to increase the spatial and temporal density of outdoor air quality measurements when integrated with an internet of things (IoT) system that is able to report sensor data in near real-time. Many low-cost particle sensors are currently available, but there are serious concerns about data accuracy and precision, sensor reliability, and suitability for outdoor deployment. We evaluate a newly available, low-cost particle sensor from Sensirion AG, which reports having high accuracy with other desirable capabilities, including low power consumption, for the ability for long-term sensor deployment, and measurement of particulate matter (PM) size speciation with number concentration, for less than \$50/sensor.

This talk will discuss the testing of this new PM sensor in a laboratory setting, efforts to develop an IoT system for outdoor deployments, and the evaluation of this sensor to collect measurements of outdoor PM levels. In all tests, the new sensor was compared to measurements from a DustTrak-DRX Model 8533, and in some tests, to a condensation particle counter and an ARISense measurement system. Laboratory calibration used particles of known size (PM₁, PM_{2.5}, etc.) at various number concentrations (spanning 10² to 10⁴ cm⁻³). Outdoor testing demonstrates performance over a range of airborne PM levels in a relatively humid, rural environment. Time-series plots reveal general agreement in short-term PM variability captured by both sensors; however, consistent differences in absolute values reveal that offsets may be required. Time-series analysis techniques are compared to identify similarities between tested sensor output, while spatial interpolation of averaged and event-specific data is used to build maps of PM levels.

13AS.3

Evaluating Performance of High-, Mid-, and Low-cost Analyzers for Capturing Heavy-duty Diesel Truck Exhaust Plumes. REBECCA SUGRUE, Chelsea V. Preble, Thomas W. Kirchstetter, *University of California, Berkeley*

Studies of in-use truck emissions typically employ expensive, regulatory-grade analyzers. However, there is a growing interest in using low-cost sensors in this field—for example, as a widely deployed surveillance tool that could efficiently identify high-emitting trucks that may need maintenance. To date, there has been little to no evaluation of low-cost sensor performance for truck exhaust plume capture, which requires fast and accurate analyzer response of rapidly changing pollutant concentrations when trucks pass by.

This study evaluates the performance of high-, mid-, and low-cost analyzers for measurement of exhaust plumes from trucks that pass by a fixed sampling location. This performance is based on resulting fuel-based black carbon (BC) emission factors determined with a carbon balance method. At a terminal entrance at the Port of Oakland, we measured BC emission rates from 888 in-use drayage trucks using a suite of four different BC and four different carbon dioxide (CO₂) analyzers. This suite of analyzers generated 16 BC emission factors for each truck that was sampled. We considered the precision of the analyzers and the resulting limit of detection for near-zero emission factors. These data also provided a basis for evaluating the ability of each analyzer pairing to identify the highest emitting trucks that account for most of the fleet's pollution. There was a strong correlation in emission rates calculated with the highest and lowest cost CO₂ analyzers. This agreement indicates that the low-cost option is a reliable alternative. The distributions of BC emission factors computed with various pairs of high- and low-cost BC and CO₂ analyzers are very similar. However, we found that many of the trucks identified as higher emitters with a pair of high-cost BC and CO₂ analyzers were not identified as higher emitters with other analyzers.

13AS.4

Evaluation of Low-Cost PurpleAir Monitors and In-Field Correction Using Co-Located Portable Filter Samplers. JESSICA TRYNER, Christian L'Orange, John Mehaffy, Dan Miller-Lionberg, Josephine Hofstetter, John Volckens, *Colorado State University*

Low-cost aerosol monitors have the potential to provide more spatially- and temporally-resolved data on ambient fine particulate matter (PM_{2.5}) concentrations than are typically available from regulatory monitoring networks; however, low-cost monitors—which do not measure PM_{2.5} mass directly and tend to be sensitive to variations in particle size and refractive index—sometimes produce inaccurate estimates of PM_{2.5} concentrations. In this study, we investigated laboratory- and field-based approaches for calibrating low-cost monitors against gravimetric filter samples. First, we investigated the PurpleAir response to NIST Urban PM and derived a laboratory-based gravimetric correction factor. Then, we co-located PurpleAir monitors with compact, portable filter samplers at 15 outdoor sites spanning a 3×3-km area in Fort Collins, Colorado. We evaluated whether PM_{2.5} correction factors derived from periodic co-locations with portable filter samplers improved the accuracy of the PurpleAir monitors (relative to reference filter samplers operated at 16.7 L·min⁻¹). The atmospheric (ATM) PM_{2.5} concentrations reported by the PurpleAir monitors appeared to increase linearly with the concentration of NIST Urban PM measured by a TEOM, but neither the factory ATM calibration nor the laboratory-based correction factor translated to the field. Correction factors derived in the field from monthly, weekly, semi-weekly, and concurrent co-locations with portable filter samplers increased the fraction of 72-hour average PurpleAir PM_{2.5} concentrations that were within 20% of the concentration measured using the reference filter sampler from 15% (for uncorrected measurements) to 45%, 59%, 56%, and 70%, respectively. In addition, 72-hour average PM_{2.5} concentrations measured using the portable and reference filter samplers agreed (bias ≤ 20% for 71% of samples). These results demonstrate that periodic co-location with portable filter samplers can improve the accuracy of 72-hour average PM_{2.5} concentrations reported by PurpleAir monitors.

13AS.5

Evaluation of Low-Cost Particulate Matter Sensors in a Test House. JONATHAN GINGRICH, Sameer Patel, Elizabeth Graham, Erin K. Boedicker, Delphine K. Farmer, Richard Corsi, Marina Vance, *University of Colorado Boulder*

Exposure to particulate matter (PM) causes a wide spectrum of health effects¹. There are many sources of indoor PM resulting in potentially high exposures to humans. Because of this and because humans spend most of their times indoors, indoor concentration measurements are important for assessing potential exposure and resulting health effects. Recently, low-cost air quality instruments marketed for consumers have become popular for measuring indoor air quality and contaminant levels by homeowners. We tested five popular commercially-available indoor air quality instruments (Air Quality Egg, Dylos, PurpleAir, Speck) as well as two prototypes developed by universities (Washington University in St. Louis and Harvard) and compared them to research- and industry-grade monitors (TSI Aerodynamic Particle Sizer (APS 3321), TSI DustTrak 8520, and Handix Scientific Portable Optical Particle Sizer (POPS)) in a three bedroom manufactured test house during the HOMEChem (House Observations of Microbial and Environmental Chemistry) campaign.

Five different categories were used to test: (1) accuracy during collocation, (2) time resolution to peaks, (3) accuracy at baseline, (4) accuracy during peaks, and (5) spatial variability of responses. In general, sensors performed well at baseline. PurpleAir and Air Quality Egg agreed best with the reference monitors during collocation. At high concentrations, almost all sensors overestimated PM concentrations compared to the reference monitors. Time response varied greatly based on the resolution of the monitors. Finally, for spatial variation, almost all sensors had lower concentrations in the living room than in the kitchen during cooking events, showing the spatial variability of PM during these events. While low-cost optical sensors show some ability to respond to peaks and are close to reporting an accurate PM concentration at the baseline, their considerable overestimation during peaks show that more development is needed before they can be considered accurate and robust sensors for consumers.

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13BA.1

Evaluation of Five Samplers to Determine Personal Bioaerosol Exposure in Indoor and Outdoor Environments. NIRMALA THOMAS, Taewon Han, Hyeon-Ju Oh, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

Four existing personal aerosol and bioaerosol samplers and one newly-developed personal bioaerosol sampler were used to determine personal exposures to bioaerosols at three distinctly different locations. Personal Electrostatic Bioaerosol Sampler (PEBS) was the in-house sampler developed at Rutgers University, and the other samplers were CIP 10-M sampler (Air Sampling Devices, Milford, NH), Ultrasonic Personal Aerosol Sampler (UPAS; Access Sensor Technologies, Fort Collins, CO), NIOSH Personal Bioaerosol Cyclone Sampler 251 (NIOSH, USA) and Button Aerosol Sampler (SKC, Inc., Eighty Four, PA). The sampling locations included outdoors, a horse barn, and a greenhouse on Rutgers Cook campus. These locations had different wind speeds, temperature, relative humidity, and local microenvironments. Two sets of all five samplers were placed on the chest of two mannequins to represent sampling from an individual's breathing zone, and samples were collected twice at each location. Total bacteria and fungi were counted by epifluorescence microscope and hemocytometer chamber, while culturable bioaerosols were determined by plating. Viable bioaerosols were detected using bioluminescence of adenosine triphosphate (ATP) and cFDA-AM/Propidium Iodide cell viability assays. The measured ATP concentrations varied from 10^3 to 10^6 Relative Luminescence Units (RLU)/m³. PEBS had the highest percentage of live/viable cells (mean fraction: $40 \pm 4\%$; $p < 0.05$). However, the injured cell percentages did not vary significantly between the samplers. The highest culturable concentrations of bacterial and fungal cells were collected by NIOSH sampler, but it was not statistically different from that measured by PEBS and Button samplers ($p > 0.05$). Our results suggest that personal samplers' collection mechanism and sample retrieval techniques affected their ability to measure bioaerosols accurately.

13BA.2**Development of Antimicrobial Resistance in Bioaerosols.**

Gabriela Ramos, Brinda Venkateshaiah, Ryan Gerlich, Anish Jantrania, MARIA KING, *Texas A&M University*

The objective of this study is to focus on the microbial evolution as bacteria are aerosolized from contaminated bodies of water. In this case, the aerosols are released from different septic tanks located at a rural area in Texas. The septic tanks are connected by a filtration system; the first septic tank being the most contaminated and fourth septic tank being the most purified. Air and water were collected at each septic tank during two seasons, in the winter and summer. Samples from each tank were taken with open and closed lids to observe the effect it may have on the concentration of bioaerosols. The water inside each septic tank was also sampled to compare the concentration of microorganisms in the water to the concentration of microorganisms in the bioaerosol samples. The results of the culturable counts and quantitative Polymerase Chain Reaction (qPCR) confirmed that the concentration of bacteria aerosolized is less than the concentration of bacteria in water, however there were still significant numbers of bioaerosols detected around the septic tanks. Microbiome analysis showed that the majority of the bioaerosols come from the water. The Kirby Bauer analysis concluded that the water samples had higher numbers of antimicrobial resistant bacteria compared to the bioaerosols. The highest percentage of antimicrobial resistance in the bioaerosol samples was 50%. Although low in comparison to the higher 87.5% resistance of the water samples, the antimicrobial resistance in bioaerosols caused by the aerosolization of pathogens can potentially be hazardous to human health if inhaled, ingested, or absorbed through the skin.

In conclusion, lower numbers of aerosolized bacteria were collected during the winter sampling compared to the bacteria concentration in water. Bioaerosols are exposed to different stresses including colder temperatures, desiccation, and lack in nutrients that could lead to the development of antimicrobial resistance.

13BA.3**Antibiotic Resistance Genes Distribution Analysis in Common Respiratory Pathogens.** MINFEI WANG, Maosheng Yao, *Peking University*

Abstracts:Respiratory infection affects millions of lives worldwide every year. The transmissions of airborne pathogens and antibiotic resistance genes (ARGs) make the situation even worse. Certain bacterial pathogens such as *Pseudomonas aeruginosa*, *Haemophilus influenza* and *Methicillin-resistant Staphylococcus aureus (MRSA)* can be exhaled out from the infected patients. On the other hand, antibiotic resistance genes (ARGs) in ambient particulate matters have emerged as an increasing global health concern. However, the resistance mechanisms of respiratory pathogens remain to be incompletely understood, which may aggravate the misuse of antibiotics. In this study, the levels of 39 ARG subtypes resistant to seven common classes antibiotics such as quinolones, β -lactams, macrolides, tetracyclines, sulfonamides, aminoglycosides and vancomycins and two mobile genetic elements (MGE) including *tnpA* encoding transposase and *intl1* encoding integrase class I in *P.aeruginosa*, *H. influenzae* and MRSA were screened. The antimicrobial susceptibility test was conducted to further explore the expression of ARG subtypes detected in *P. aeruginosa*. The results indicated that the Quinolone resistance gene *qepA* (99.90%) the Tetracycline gene *tetC* (99.97%) and the Macrolide resistance gene *ermC* (70.14%) were the most abundant ARG subtypes in *P. aeruginosa*, *H. influenza* and MRSA, respectively. Overall, here we intended to profile the ARG subtypes distribution and to explore the ARGs expression levels in several common respiratory pathogens, which could be useful for the antibiotic therapy guidance and might alleviate the social panic of ARGs in ambient environment.

Keywords: antibiotic resistance genes; distribution; respiratory pathogens; *Pseudomonas aeruginosa*

13BA.4

Quantitative Microbial Exposure Assessment of Aerosolized Enteric and Opportunistic Pathogens in La Paz, Bolivia: A One Health Approach to Study Bioaerosols in Cities with Poor Sanitation. LUCAS ROCHA-MELOGNO, Olivia Ginn, Emily Bailey, Gregory Gray, Michael Bergin, Freddy Soria, Marcos Andrade, Joseph Brown, Marc Deshusses, *Duke University*

In an increasingly urbanized world, many cities in developing countries have little to no safely managed sanitation services. Their citizens consequently are exposed to a variety of fecal pathogens through various pathways, posing significant human health risks. Cities with open sewers are of particular interest to us because we hypothesize that aerosolized fecal pathogens pose a risk of infection in such contexts, potentially creating lifetime health deficits. The goal of our field study was to explore two exposure pathways in an environment where harmful and opportunistic bioaerosols may be prevalent.

The city of La Paz in Bolivia extends in a canyon with poor urban planning and discharges its industrial wastewater, hospital and domestic sewage into the Choqueyapu River. We conducted passive and active bioaerosol sampling at multiple sites next and at <5 km away from the Choqueyapu River hypothesized to be a source of bioaerosols during the rainy and dry season in 2019. We took minute-interval measurements of wind speed, temperature, relative humidity, UV index and PM_{2.5} (using low-cost sensors) to evaluate their impact in the bioaerosols fate and transport. Molecular analyses were conducted on samples brought back to the US using RT-PCR and dd-PCR to identify and quantify gene abundance of pathogens of interest. During the rainy season, an average airborne concentration of 53 total coliform (TC) CFU/m³ was found, with up to 19% of them being viable *E. coli*. Settle-plate fluxes averaged 130 TC CFU/m²/h and only one *E. coli* CFU was observed (n=60 plates). Distance from the Choqueyapu River did not have an effect on the CFU fluxes observed throughout the city except in one site. In this talk, detailed findings and exposure analyses combining our expertise in microbiology, air pollution and epidemiology will be presented.

13BA.5

Biological Composition of Coastal Airborne Particulate Matters during Enteromorpha Prolifera Outbreak. JIAHUI RONG, Song Yu, Yan Wu, *Shandong University*

The effects of Enteromorpha Prolifera Outbreak on coastal airborne particles were investigated in the paper. Air samples were collected using HighBioTrap sampler operated at its standard flow rate of 1000 L/min at different distances (0m, 500m, 1000m) from the seacoast before, during and after the Enteromorpha Prolifera Outbreak. Offshore seawater samples from the same period were also collected. Microbial communities, antibiotic and heavy metal resistance genes, allergens, endotoxins as well as marine algae toxins were analyzed for both air and seawater samples. Results showed that the fungal concentration and diversities in the coastal air were significantly higher during the Enteromorpha Prolifera Outbreak than other two phases. In contrast, which were opposite to bacterial ones. The bacterial DNA concentrations and diversities in the coastal airborne particulates showed an onward trend, while the fungi showed a downward trend. Compared with seawater without Enteromorpha Prolifera, there were more antibiotic and heavy metal resistance genes in atmospheric particles during the outbreak of Enteromorpha Prolifera. And Transposase *tnpA* and vancomycin resistance genes (*vanB* and *vanRA*) were only detected for air samples collected during the Enteromorpha Prolifera Outbreak. The results from this study provide further new information in biological composition of coastal airborne particulate matters during Enteromorpha Prolifera Outbreak.

13CA.1

Chemical Evolution of Particulate and Gas-phase Emissions from Meat Cooking. AIKATERINI LIANGO, Spiro Jorga, Christos Kaltsonoudis, Antonios Tasoglou, Leif Jahn, Mingyi Wang, Spyros Pandis, *Carnegie Mellon University, University of Patras*

Cooking organic aerosol (COA) can be a significant component of fine particulate matter since it can contribute up to 30% of the ambient PM₁ in urban areas (Sun et al., 2011; Crippa et al., 2013). While the fresh cooking emissions have received considerable attention, there is little information about their chemical evolution in the atmosphere.

Cooking emissions from charbroiled hamburgers were injected in a 10 m³ Teflon smog chamber. After a characterization phase the emissions were exposed to ozone and/or OH radicals. A High Resolution Time-of-Flight Aerosol Mass Spectrometer (AMS) together with a Scanning Mobility Particle Sizer (SMPS) were continuously monitoring the aerosol number and composition. The black carbon concentration was measured with a Photoacoustic Extinctionmeter and was around 1% of the total PM₁ in all experiments. The AMS and the SMPS time series were corrected for particle wall losses using the method of Wang et al. (2018). Our results showed that even the organic particle O:C increased by around 50% during aging, there was little additional particulate mass produced. The concentration of the organic compounds in the gas phase during the experiments were measured with a Time-of-Flight Chemical Ionization Mass Spectrometer (ToF-CIMS) with iodine as a reagent ion as well as a Time-of-Flight Proton Transfer Reaction Mass Spectrometer (PTR-TOFMS). A number of saturated and unsaturated fatty acids were detected and the temporal evolution of their concentrations during the chemical aging phase was investigated.

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13CA.2

Laboratory Chamber Study on Organic Acids Production from Biogenic VOC Oxidation. YUNLE CHEN, David Tanner, Greg Huey, Rodney J. Weber, Nga Lee Ng, *Georgia Institute of Technology*

Organic acids are ubiquitous in the atmosphere. They constitute an important fraction of atmosphere organic carbon and can play a role in aerosol chemistry. Recent studies have shown that the sources of atmospheric organic acids (e.g. formic and acetic acid) are largely underestimated by models, and the oxidation of biogenic volatile organic compounds (VOC) can be a predominant source of organic acids. Meanwhile, the formation pathway of organic acids in biogenic VOC oxidation remains largely unexplored.

In this study, we conducted a series of laboratory experiments at the Georgia Tech Environmental Chamber (GTEC) facility to investigate the formation and evolution of organic acids from oxidation of biogenic VOC (α -pinene and isoprene) under various conditions. Gas- and particle-phase organic acids were monitored by a chemical ionization mass spectrometer (CIMS) using SF₆⁻ as reagent ion and a Particle-into-Liquid Samplers coupled with ion chromatographs (PILS-IC), respectively, allowing for an inclusive measurement of organic acid yields and gas-particle partitioning. Aerosol composition were comprehensively characterized using a High-Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS) and a HR-ToF-CIMS coupled with a Filter Inlet for Gases and AEROSols (FIGAERO). The roles of water vapor and aerosol liquid water content are investigated specifically. We found that the formation of organic acids is largely dependent on water abundance and the corresponding yields and mechanisms will be discussed.

13CA.3

Influence of Ammonia and Relative Humidity on the Optical Properties of Secondary Organic Aerosol Particles. YUMENG CUI, Alexander Frie, Isis Frausto-Vicencio, Francesca Hopkins, Roya Bahreini, *University of California, Riverside*

To understand the radiative impacts of secondary organic aerosol (SOA) particles, it is important to know their optical properties. In this work, we investigate the impact of ammonia (NH_3) at different relative humidity (RH) levels on SOA optical properties. For this investigation, SOA was produced by reacting 1-methylnaphthalene or longifolene, with hydroxyl radicals under variable nitric oxide, RH, and NH_3 conditions. During SOA formation, the chemical composition and optical properties of SOA were monitored. In addition, single scattering albedo (SSA), mass absorption coefficient (MAC), and refractive index (RI) of SOA at $\lambda=375$ nm were calculated.

At low RH ($< \sim 30\%$) and in the presence of NH_3 , longifolene SOA had relatively high SSA values and low absorption coefficients (β_{abs}) under both intermediate- and high- NO_x regimes. This suggests that longifolene SOA is mostly scattering. In 1-methylnaphthalene experiments, β_{abs} increased soon after initiation of the experiment, and the resulting SSA and MAC values suggest the formation of light-absorbing aerosols (with $\text{MAC}_{\text{max}} \approx 0.3\text{-}0.4$ m^2/g). The chemical composition of SOA will be analyzed, and results about the organic and nitrate fraction in aerosols along with the contribution of organic nitrates will be related to the SOA optical properties. To better understand the role of NH_3 under different conditions, results from experiments at higher RH (60%-70%) will also be provided.

13CA.4

Enhanced Ligand-Promoted Photochemical Reduction of Ferric Iron by Carbonaceous Nanoparticles. Ashleen Reddy, ANNE JOHANSEN, *Central Washington University*

Iron (Fe) is a limiting nutrient in many parts of the open ocean where atmospheric deposition of Fe-containing aerosol particles may constitute the main source. Although only a small portion of the total aerosol Fe is available for biological uptake, also referred to as the soluble fraction, the mechanisms that control Fe solubility in the atmosphere and surface ocean remain elusive. Here, we focus on atmospheric processes that may contribute to the larger relative soluble Fe concentrations observed in combustion-derived aerosol particles compared to those seen in their crustal counterparts. Laboratory experiments were conducted on acidic slurries of ferrihydrite in the presence of oxalate and various carbonaceous nanoparticles (CNPs), in dark and under simulated solar radiation. Ferrous (Fe(II)) and reducible-ferric iron (Fe(III)), and oxalate were analyzed throughout the experiment using UV-Vis spectrophotometry and ion chromatography, respectively. Results show that under solar radiation, CNPs contribute to increases in (i) Fe(II) production by a factor of up to 5.5, and (ii) reducible-Fe(III) production by a factor of 27 relative to experiments in the absence of CNPs. Generally, Fe(II) constitutes between 61 and 91% of the combined Fe forms quantified. Thus, the presence of CNPs, including soot, seems to facilitate the ligand-promoted photochemical reduction of Fe(III), thereby providing a potential mechanism that explains the higher fractional Fe solubility seen in combustion-derived aerosol particles.

13CA.5

Ocean Biology Effects on Saccharide Composition in Sea Spray Aerosol. ELIAS HASENECZ, Wyeth Gibson, Samantha Kruse, Jon Sauer, Kathryn Mayer, Chris Lee, Kimberly Prather, Elizabeth Stone, *University of Iowa*

Ocean biology impacts the chemical composition of sea spray aerosol (SSA) and consequently properties like cloud formation. Saccharides comprise a significant portion of SSA organic mass and are examined to evaluate how ocean biology impacts SSA's physicochemical properties. Sub and supermicron SSA was collected during two phytoplankton blooms, one with added heterotrophic bacteria. Saccharides were hydrolyzed, then separated and quantified by high performance ion chromatography with pulsed amperometric detection. Peak total saccharide concentrations were similar across the two mesocosm experiments and decreased in SSA after the phytoplankton bloom by a factor of up to 8.5. This decrease was more prominent by a factor of two times in bacteria spiked mesocosms suggesting added bacteria overall decreased saccharide levels by scavenging. This decrease was greatest for glucose (by 3.5 times), suggesting that glucose was readily scavenged by bacteria. In contrast, the decrease in galactose concentrations after the phytoplankton bloom was not enhanced by the bacteria addition, which is attributed to its presence in less labile polymeric materials. Although arabinose is associated with bacterial activity, there was no significant increase in its' concentrations across two mesocosms. Instead, arabinose concentration decreased following the total saccharide trend. This finding suggests that the scavenging of arabinose outweighed release by plankton and bacteria. The observed temporal trends in saccharide levels in SSA are being further examined with respect to saccharide monomer concentrations in sub-surface water, fractionated by size using ultra-filtration. Measurements of inorganic ions will be used to examine the enrichment of saccharides and divalent cations in SSA under varying biological conditions.

13IS.1

Dynamic Equilibria of Volatile Chemicals between Indoor Surfaces and Indoor Air. JONATHAN ABBATT, Douglas Collins, Chen Wang, *University of Toronto, Canada*

Molecules that are viewed as volatile under outdoor conditions exhibit semi-volatile behavior indoors, given the very high surface areas available in the environments in which we spend much of our time. This behavior has been demonstrated through short-term ventilation experiments in two houses, one in Texas as part of the HOMEChem field campaign and one in Toronto. For a variety of acids (HNCO, HONO and carboxylic acids with 1 to 9 carbons), the same behavior was observed: The signals dropped upon ventilation as outdoor air filled the space, followed by a rapid rise of signal after the windows and doors were closed which is indicative of re-partitioning of surface-sorbed molecules to the gas phase. The timescales of this response will be discussed as an indication of the labile nature of these sorbed species. The likelihood of partitioning to either organic- or water-rich media on the surfaces will be examined using thermodynamic partitioning modeling. Further consequences of this partitioning behavior in terms of surface reactions will also be discussed.

13IS.2

Influence of Gas-Phase and Heterogeneous OH Aging Reactions on Indoor Organic Aerosol Loading and SOA Formation. BRYAN CUMMINGS, Michael Waring, *Drexel University*

Organic aerosols (OA) continually undergo chemical aging transformations via oxidation reactions, for instance with hydroxyl radicals (OH). Broadly, these transformations include molecular functionalization and fragmentation. OA is a system with particle-bound organic material (OM) and gaseous OM in a state of thermodynamic gas-to-particle equilibrium. OM in either phase may undergo transformations, causing their volatility and degree of oxygenation to change, potentially increasing or decreasing the condensed OA concentration (C_{OA}). The two-dimensional volatility basis set (2D-VBS) constrains OM volatility and degree of oxygenation, models how each change throughout OH aging processes, and also predicts thermodynamic partitioning and resulting C_{OA} . Potential OA aging impacts were assessed by using the 2D-VBS framework within a larger indoor chemistry model which also predicts the indoor ozone and OH concentrations, oxidation of volatile organics, secondary OA (SOA) formation, and OA by indoor emissions and outdoor-to-indoor transport. Using input distributions characteristic of U.S. residences, indoor OH was predicted as not typically high enough to meaningfully impact C_{OA} by aging processes on a daylong time-averaged basis (increases of <5%). However, reasonable and individual circumstances were modeled where OA transformations due to OH-induced aging accounted for increases in C_{OA} of ~30%. One such case was a room where ample sunlight led to a high temperature and generation of OH by photolytic reactions with nitrous acid (HONO) sourced from indoor surfaces. High temperatures encourage more OM to exist in the gas phase where it more quickly reacts with OH (compared to heterogeneous reactions) and subsequently may condense into the particle phase. Additionally, simulated terpene-based cleaning events led to similar increases in OA due to OH-induced aging. These results will be discussed.

13IS.3

Investigation of Natural Ventilation and Household Activities during the Air Composition and Reactivity from Outdoor and Indoor Mixing (ACRONIM) Field Campaign. CLAIRE FORTENBERRY, Michael Walker, Audrey Dang, Azin Eftekhari, Arun Loka, Gauri Date, Karolina Cysneiros de Carvalho, Glenn Morrison, Brent Williams, *Washington University in St Louis*

The Air Composition and Reactivity from Outdoor and Indoor Mixing (ACRONIM) field campaign was launched to investigate the influence of natural ventilation (i.e., window opening to regulate temperature) on indoor air quality. This study was conducted in two phases in two distinct St. Louis, MO area homes and featured a suite of instruments to characterize chemical and physical properties of indoor particles and gases. In particular, a Thermal desorption Aerosol Gas chromatograph (TAG) provided phase partitioning approximations for key semi- and intermediately volatile organic compounds (S/IVOCs) with approximately four-hour time resolution. During the first phase of the campaign, we examined several distinct chemical and physical processes occurring inside the home as windows are opened. While volatile gases were primarily affected by dilution as windows were opened, many S/IVOCs were enhanced in the gas phase and subsequently partitioned to the particle phase as higher air change rates drove increased volatilization from surface films. Increased outdoor ventilation with window opening also drove higher indoor concentrations of particles and oxidants (e.g., ozone). An increase in indoor ozone concentrations subsequently promoted formation of oxidized species from surface and gas-phase reactions, though compounds expected to react significantly with ozone (e.g., monoterpenes) were primarily affected by dilution from the increased ventilation rate.

These chemical and physical processes driven by natural ventilation were investigated within an unoccupied test home. However, occupant behavior will influence the degree to which each process impacts indoor air quality. Here, we present results from special experiments conducted during the occupied periods of both phases of the ACRONIM campaign, wherein researchers participated in common household activities such as cooking and cleaning. Specifically, we investigate how natural ventilation and occupant behavior interact to influence particle resuspension, S/IVOC phase partitioning, and particle- and gas-phase oxidative chemistry.

13IS.4

Indoor Abundance of Semivolatile Organic Compounds under Dynamic Aerosol Conditions. DAVID LUNDERBERG, Kasper Kristensen, Yilin Tian, Caleb Arata, Yingjun Liu, Pawel Misztal, William Nazaroff, Allen Goldstein, *University of California, Berkeley*

The chemical composition of indoor environments is not fully understood; nor are the processes and emission sources controlling that composition. Implementing high-time resolution measurements of airborne organics in residential environments can contribute to a better understanding of the dynamic processes affecting the air we breathe. Semivolatile thermal desorption aerosol gas chromatography (SV-TAG) quantifies the speciated abundance and gas-particle phase-partitioning of compounds with vapor pressures between $\sim C_{14}$ and $\sim C_{30}$ alkanes at hourly time-resolution. We present data acquired by SV-TAG during two separate field campaigns that investigated residential indoor air under controlled conditions (HOMEChem campaign: manufactured test house in Austin, Texas) and normal-occupancy conditions (H2 campaign: single-family residence in Orinda, California).

The indoor airborne composition of semivolatile organic compounds (SVOCs) is chemically complex, with significant contributions from outdoor air, indoor building materials, and occupant-driven perturbations. Because SVOCs exist in multiple phases throughout a residence, including in dust, in surface films, in airborne particulate matter, and in the gas-phase, changes in aerosol properties can induce shifts in partitioning, including in the relative abundance of species that are surface-sorbed rather than airborne. Outdoor infiltration of particulate matter and emissions from cooking events can introduce airborne particles into the indoor environment. The impact of these aerosol sources on SVOC partitioning phenomena was studied during the HOMEChem and H2 campaigns. Analysis of vacant periods, when particles are expected to be of primarily of outdoor origin, were compared against periods influenced by indoor cooking events. During the HOMEChem campaign, concentration enhancements of SVOCs from cooking events consisted of gas- and particle-phase species directly attributable to the cooking process and by lower-volatility species related to primary emissions from building materials.

13IS.5

Molecular Composition and Gas-Particle Partitioning of Indoor Cooking Aerosol: Insights from a FIGAERO-CIMS. CATHERINE MASOUD, Dongyu S. Wang, Lea Hildebrandt Ruiz, *University of Texas at Austin*

The average American spends most of their life indoors, highlighting the importance of studying indoor air pollutants. The House Observations of Microbial and Environmental Chemistry (HOMEChem) field campaign focused on the effects of cooking, cleaning, and occupancy-related activities in a home. Here, we present our analyses of the data collected during cooking events, which resulted in the highest observed organic aerosol concentrations. Using a Filter Inlet for Gases and Aerosols mounted onto a High-Resolution Time-of-Flight Chemical Ionization Mass Spectrometer (FIGAERO-CIMS), we identify over 400 compounds using high-resolution peak fitting and propose their chemical identities and sources. We then categorize them under (1) cooking-related emissions (2) industrial emissions (phthalates, phosphanes, organosulfates, etc.), (3) personal care products, and (4) others. We also identify “chemical markers” for some of the cooking events – for example we observed elevated paradol levels (from ginger), and levoglucosan and isomaltol levels (from caramelization of sugar) when a sweet potato casserole was prepared.

We use the ratio of gas and particle-phase signals obtained from the FIGAERO-CIMS to calculate a partitioning fraction, and convert species-specific partitioning fractions to saturation concentration values. We compare these values to saturation concentration values obtained from parameterizations based on elemental composition (Li et al., 2016). We find that while there is substantial correlation between the calculated (via volatility parameterizations) and measured (using the FIGAERO-CIMS instrument) saturation concentrations, the volatility parameterization method consistently gives higher values than those obtained from the FIGAERO. We suggest potential reasons for this difference and compare different methods for obtaining volatility information from a FIGAERO-CIMS.

[1] Li, Y., Pöschl, U., & Shiraiwa, M. (2016). Molecular corridors and parameterizations of volatility in the chemical evolution of organic aerosols, 3327–3344. <https://doi.org/10.5194/acp-16-3327-2016>.